

EXTENSIONS OF SYMMETRIC OPERATORS I: THE INNER CHARACTERISTIC FUNCTION CASE.

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ABSTRACT. Given a symmetric linear transformation on a Hilbert space, a natural problem to consider is the characterization of its set of symmetric extensions. This problem is equivalent to the study of the partial isometric extensions of a fixed partial isometry. We provide a new function theoretic characterization of the set of all self-adjoint extensions of any symmetric linear transformation B with equal indices and inner Livsic characteristic function Θ_B by constructing a natural bijection between the set of self-adjoint extensions and the set of all contractive analytic functions Φ which are greater or equal to Θ_B . In addition we characterize the set of all symmetric extensions B' of B which have equal indices in the case where Θ_B is inner.

1. INTRODUCTION

The purpose of this paper is to study of the family of all closed symmetric extensions of a given closed simple symmetric linear transformation B with equal deficiency indices (n, n) , $1 \leq n < \infty$ defined on a domain in a separable Hilbert space in the case where the Livsic characteristic function of B is an inner function. For $n \in \mathbb{N} \cup \{\infty\}$, $\mathcal{S}_n(\mathcal{H})$ will denote the set of all closed simple symmetric linear transformations with indices (n, n) defined in a separable Hilbert space \mathcal{H} . More generally \mathcal{S}_n will denote the family of all closed simple symmetric linear transformations with indices (n, n) defined in some separable Hilbert space, and \mathcal{S} the set of all closed simple symmetric linear transformations with equal indices defined in some separable Hilbert space.

If A is a symmetric linear transformation which extends $B \in \mathcal{S}_n(\mathcal{H})$ and $\text{Dom}(A)$ is also contained in \mathcal{H} then we call A a canonical extension of B . If, on the other hand A is symmetric in \mathcal{K} where $\mathcal{K} \supsetneq \mathcal{H}$, then we call A a non-canonical extension of B . The set of all canonical extensions of B can be completely characterized by the set of all partial isometries between the deficiency subspaces $\text{Ker}(B^* - i)$ and $\text{Ker}(B^* + i)$, see for example [1, Chapter VII]. Our goal is to provide a new characterization the set of extensions, canonical and non-canonical in the special case where the characteristic function Θ_B is inner. (Recall that in this case B is unitarily equivalent to multiplication by z in a model subspace $K_{\Theta_B}^2 = H^2(\mathbb{C}_+) \ominus \Theta_B H^2(\mathbb{C}_+)$ of Hardy space [2, 3, 4].)

We will begin with the study of the self-adjoint extensions of B , denoted $\text{Ext}(B)$, and show that there is a bijective correspondence between $A \in \text{Ext}(B)$ and the set of all contractive analytic (matrix) functions Φ_A which obey:

$$\Phi_A \geq \Theta_B,$$

see Theorem 8.14. Here, given contractive analytic matrix functions Φ, Θ on \mathbb{C}_+ , we say that $\Theta \leq \Phi$ provided that $\Theta^{-1}\Phi$ is contractive and analytic on \mathbb{C}_+ . This provides an alternative to the classical results of M.G. Krein (see *e.g.* [5, Theorem 6.5] for the $(1, 1)$ case) which are formulated in terms of generalized resolvents and R -functions. Our characterization has the advantage of providing a

natural function-theoretic connection between the Livsic characteristic function of $B \in \mathcal{S}$ and the set of its self-adjoint extensions.

We will also study a natural partial order on \mathcal{S} : we say that $B_1 \lesssim B_2$ for $B_1, B_2 \in \mathcal{S}$ if $B_1 \simeq B'_1 \subset B_2$, where \simeq denotes unitary equivalence and we use the \subset notation to denote when one linear transformation is an extension of another. In words, B_1 is less than or equal to B_2 if B_2 is an extension of B'_1 where B'_1 is unitarily equivalent to B_1 . Application of the Cayley transform, which is a bijection from \mathcal{S} onto \mathcal{V} , the set of all partial isometries with equal indices, converts this into a partial order on \mathcal{V} . Modulo unitary equivalence, this is the same as the partial order previously defined by Halmos and McLaughlin on partial isometries in [6]. In the case where Θ_{B_1} is an inner function, we provide necessary and sufficient conditions on Θ_{B_2} so that $B_1 \lesssim B_2$ in Theorem 9.5.

Many of these results will be achieved using the concept of a generalized model. This is a reproducing kernel Hilbert space theory approach which generalizes the concept of a model for a symmetric operator as defined in [4].

2. PRELIMINARIES

Recall that a linear transformation B is simple, symmetric and closed with deficiency indices (n, n) if it is defined on a domain $\text{Dom}(B)$ contained in a separable Hilbert space \mathcal{H} and has the following properties:

$$\langle Bx, y \rangle = \langle x, By \rangle, \quad \forall x, y \in \text{Dom}(B), \quad B \text{ is symmetric}; \quad (2.1)$$

$$\bigcap_{z \in \mathbb{C} \setminus \mathbb{R}} \text{Ran}(B - z) = \{0\}, \quad B \text{ is simple}; \quad (2.2)$$

$$\{(x, Bx) \mid x \in \text{Dom}(B)\} \text{ is a closed subset of } \mathcal{H} \oplus \mathcal{H}, \quad B \text{ is closed}; \quad (2.3)$$

$$n_- := \dim \left(\text{Ran}(B - i)^\perp \right) = n = \dim \left(\text{Ran}(B + i)^\perp \right) =: n_+, \quad (2.4)$$

$B \text{ has equal deficiency indices } (n_+, n_-).$

Condition (2.2) can be restated equivalently as: B is simple if and only if there is no non-trivial subspace reducing for B such that the restriction of B to the intersection of its domain with this subspace is self-adjoint. For many of our results we will need to assume that $n < \infty$ is finite.

A partial isometry V is called simple, or c.n.u. (completely non-unitary) if it has no unitary restriction to a proper (and non-trivial) reducing subspace. The deficiency indices for V are the pair of non-negative integers (n_+, n_-) defined by

$$n_+ := \dim(\text{Ker}(V)) \quad \text{and} \quad n_- := \dim \left(\text{Ran}(V)^\perp \right),$$

and it is not difficult to see that these are the same as the defect indices of V as defined in [7].

There is a bijective correspondence between $\mathcal{S}_n(\mathcal{H})$ and $\mathcal{V}_n(\mathcal{H})$ which we now describe: Given a simple symmetric linear transformation $B \in \mathcal{S}_n(\mathcal{H})$ and $z \in \mathbb{C} \setminus \mathbb{R}$, let Q_z denote the projection onto $\text{Ran}(B - \bar{z})$. The Cayley transform V_B of B is the partial isometry

$$V_B := b(B)Q_i = (B - i)(B + i)^{-1}Q_i; \quad b(z) := \frac{z - i}{z + i}, \quad (2.5)$$

where $b(B) = (B - i)(B + i)^{-1}$ is a well-defined isometry from $Q_i\mathcal{H} = \text{Ran}(B + iI)$ onto $Q_{-i}\mathcal{H} = \text{Ran}(B - i)$. Note that $\text{Ker}(V) = \text{Ran}(B + i)^\perp$ and $\text{Ran}(V)^\perp = \text{Ran}(B - i)^\perp$, and so it follows that the deficiency indices of V_B are the same as those of B .

Conversely suppose that V is a simple partial isometry on \mathcal{H} with defect indices (n_+, n_-) . One can construct a symmetric linear transformation B_V by defining

$$\text{Dom}(B_V) := (1 - V)\text{Ker}(V)^\perp,$$

and

$$B_V f = b^{-1}(V)f = i(1 + V)(1 - V)^{-1}f, \quad f \in \text{Dom}(B_V); \quad b^{-1}(z) := i \frac{1 + z}{1 - z}.$$

Again it is easy to check that B_V and V have the same deficiency indices. One can further verify that $B_{V_B} = B$ and $V_{B_V} = V$ for any symmetric linear transformation B and partial isometry V , respectively. This shows that the maps $B \mapsto V_B$ and $V \mapsto B_V$ are inverses of each other so that these maps are bijections between \mathcal{S} and \mathcal{V} . We will use this bijection between \mathcal{V} and \mathcal{S} to formulate problems in whichever setting is most convenient, and to obtain equivalent results for both classes of linear transformations.

Given $B \in \mathcal{S}_n(\mathcal{H})$, $n < \infty$, one can construct a complete unitary invariant Θ_B , called the Livsic characteristic function as follows: Pick orthonormal bases $\{u_j\}_{j=1}^n$ and $\{v_j\}_{j=1}^n$ for $\text{Ran}(B + i)^\perp$ and $\text{Ran}(B - i)^\perp$ respectively and choose arbitrary (not necessarily orthonormal) bases $\{w_j(z)\}_{j=1}^n$ for $\text{Ran}(B - \bar{z})^\perp$. Let

$$B(z) := [\langle w_j(z), u_k \rangle]_{1 \leq j, k \leq n}, \quad (2.6)$$

and

$$A(z) := [\langle w_j(z), v_k \rangle]_{1 \leq j, k \leq n}. \quad (2.7)$$

The Livsic characteristic function is then [8]

$$\Theta_B(z) := b(z)B^{-1}(z)A(z), \quad (2.8)$$

and this can be shown to be a contractive $n \times n$ matrix-valued analytic function on \mathbb{C}_+ , the upper half-plane. Note that the characteristic function Θ_B always vanishes at $z = i$. Different choices of bases in the definition yield a new characteristic function $\tilde{\Theta}_B$ which is related to the first by

$$\tilde{\Theta}_B(z) = R\Theta_B(z)Q,$$

where R, Q are fixed unitary matrices. Two Livsic characteristic functions Θ_1, Θ_2 are said to coincide or to be equivalent if they are related in this way.

For most of this paper we will assume that Θ_B is an inner function, *i.e.* Θ_B has non-tangential boundary values on \mathbb{R} almost everywhere with respect to Lebesgue measure, and these non-tangential boundary values are unitary matrix-valued. In this case $B \simeq Z_{\Theta_B}$, where $Z_{\Theta_B} \in \mathcal{S}(K_{\Theta_B}^2)$ is the symmetric operator of multiplication by z on the domain

$$\text{Dom}(Z_{\Theta_B}) = \{f \in K_{\Theta_B}^2 \mid zf \in K_{\Theta_B}^2\},$$

in the model space $K_{\Theta_B}^2 = H^2 \ominus \Theta_B H^2$, and here $H^2 = H^2(\mathbb{C}_+)$ is the Hardy space of the upper half-plane.

As shown in [4], one can also define the Livsic characteristic function for the case where $n = \infty$, and this new definition coincides with the old one for $n < \infty$. As first shown by M.S. Livsic, the Livsic characteristic function is a complete unitary invariant for $\mathcal{S}_n(\mathcal{H})$:

Theorem 2.1. *Linear transformations $B_1 \in \mathcal{S}_n(\mathcal{H}_1)$ and $B_2 \in \mathcal{S}_n(\mathcal{H}_2)$ are unitarily equivalent if and only if their characteristic functions Θ_1, Θ_2 are equivalent.*

One of the results of this paper, Theorem 8.12 will provide a similar result for all $A \in \text{Ext}(B)$. Given any $A \in \text{Ext}(B)$, we will define a characteristic function $\Phi_A = \Phi[A; B]$ which has the property that $\Lambda_A \geq \Theta_B$ where Λ_A is a Frostman shift of Φ_A vanishing at i . Theorem 8.12 will show that $\Phi_{A_1} = \Phi_{A_2}$ if and only if $A_1 \simeq A_2$ via a unitary which is the identity when restricted to \mathcal{H} .

Here is our formal definition of $\text{Ext}(B)$:

Definition 2.2. Given $V \in \mathcal{V}_n(\mathcal{H})$, let $\text{Ext}(V)$ denote the set of all unitary operators U such that

- (1) U is an extension of $V = b(B)$, i.e. $V \subseteq U$ ($U|_{\text{Ker}(V)^\perp} = V|_{\text{Ker}(V)^\perp}$) and U is unitary in some Hilbert space $\mathcal{K} \supset \mathcal{H}$.
- (2) \mathcal{K} is the smallest reducing subspace for $\text{vN}(U)$, the von Neumann algebra generated by U .

Given $B \in \mathcal{S}_n(\mathcal{H})$, we will define $\text{Ext}(B)$ to be a relabeling of the set $\text{Ext}(b(B))$. Namely if $U \in \text{Ext}(b(B))$, and $1 \notin \sigma_p(U)$, the set of eigenvalues of U , then we define A to be the self-adjoint operator $b^{-1}(U)$. If however $U \in \text{Ext}(b(B))$ and $1 \in \sigma_p(U)$, then we formally define A by $b^{-1}(U)$. In this case A is not a well defined linear transformation, it is just a renaming of $U \in \text{Ext}(b(B))$ with the understanding that $A_1 = A_2$ for $A_1 = b^{-1}(U_1)$, $A_2 = b^{-1}(U_2)$ and $U_1, U_2 \in \text{Ext}(b(B))$ if and only if $U_1 = U_2$. $\text{Ext}(B)$ is then defined to be the set of all such A . In this way there is a bijection between $\text{Ext}(b(B))$ and $\text{Ext}(B)$.

Recall that the subset notation $B \subset A$ means that A is an extension of B , i.e. $\text{Dom}(B) \subset \text{Dom}(A)$ and $A|_{\text{Dom}(B)} = B$. The subset notation $V \subseteq U$ for partial isometries V, U means that $U|_{\text{Ker}(V)^\perp} = V|_{\text{Ker}(V)^\perp}$. For simple symmetric linear transformations B_1, B_2 we have that $B_1 \subset B_2$ if and only if $b(B_1) \subseteq b(B_2)$.

Remark 2.3. If B is densely defined then every unitary extension U of $b(B)$ does not have 1 as an eigenvalue [2, Lemma 6.1.3], [9], so that every element of $\text{Ext}(B)$ is a densely defined self-adjoint operator. Note that if $A \in \text{Ext}(B)$ and $A = b^{-1}(U)$ for some $U \in \text{Ext}(b(B))$ such that $1 \notin \sigma_p(U)$, then the two conditions of the above definition are equivalent to

- (1) A is an extension of B , i.e. $B \subset A$ and A is self-adjoint in some Hilbert space $\mathcal{K} \supset \mathcal{H}$.
- (2) \mathcal{K} is the smallest reducing subspace for $\text{vN}(A)$, the von Neumann algebra generated by $b(A)$.

However if B is not densely defined, then one can find canonical unitary extensions U of $V = b(B)$ which have 1 as an eigenvalue [2, Lemma 6.1.3], [8]. In this exceptional case where U is a unitary extension of $b(B)$ and $1 \in \sigma_p(U)$, then we will always work with the unitary extension U associated with $A = b^{-1}(U)$. If $1 \in \sigma_p(U)$, one could define $A := b^{-1}(U)P_U(\mathbb{T} \setminus \{1\}) = b^{-1}(U)\chi_{\mathbb{T} \setminus \{1\}}(U)$, where χ_Ω is the characteristic function of Ω , \mathbb{T} is the unit circle and $P_U(\mathbb{T} \setminus \{1\}) = \chi_{\mathbb{T} \setminus \{1\}}(U)$ projects onto the orthogonal complement of the eigenspace to eigenvalue 1 of U . However we will have no need for this construction, and in this exceptional case where $1 \in \sigma_p(U)$ for $U \in \text{Ext}(b(B))$ we will simply work with $U \in \text{Ext}(b(B))$ instead of its inverse Cayley transform $A = b^{-1}(U)$ in $\text{Ext}(B)$. In this paper we are really studying $\text{Ext}(b(B))$, but given $U \in \text{Ext}(b(B))$ we prefer to work with $A = b^{-1}(U) \in \text{Ext}(B)$ whenever this is well-defined.

It will also be convenient to define $\text{Ext}_U(B)$ to be the set of all self-adjoint linear transformations A on \mathcal{K} for which $A \in \text{Ext}(UBU^*)$ for some isometry $U : \mathcal{H} \rightarrow \mathcal{K}$.

The set $\text{Ext}(B)$ is called the set of extensions of B . In the case where $\mathcal{K} = \mathcal{H}$, we say that A is a canonical self-adjoint extension of B . Recall that the canonical self-adjoint extensions A of B can all be obtained by first computing the Cayley transform $V := b(B)$, extending this by a *rank* $-n$ isometry $U : \text{Dom}(V)^\perp \rightarrow \text{Ran}(V)^\perp$ to obtain a unitary extension V_U of V , and then taking the inverse Cayley transform to obtain a self-adjoint linear transformation $A := b^{-1}(V_U)$.

3. LINEAR RELATIONS

In the case where B is not densely defined, its adjoint B^* is not a linear operator. Instead B^* can be realized as a linear relation, and we will discuss the basic facts about linear relations that will be needed in this section. The material from this section is taken primarily from [10] and [11, Section 1.1]. A *linear relation* L is defined to be a subspace of $\mathcal{H} \oplus \mathcal{H}$. Note that $L = \mathfrak{G}(T)$ is the graph of some closed linear operator T provided that L is closed and $(0, f) \in L$ implies that $f = 0$.

Given a linear relation L , one defines the adjoint linear relation L^* by

$$L^* := \{(g_1, g_2) \mid \langle f_1, g_2 \rangle = \langle f_2, g_1 \rangle \quad \forall (f_1, f_2) \in L\}. \quad (3.1)$$

L is called symmetric if $L \subset L^*$ and L is self-adjoint if $L = L^*$. Clearly if B is a closed symmetric linear operator with adjoint B^* then the graph, $\mathfrak{G}(B)$ of B is a closed symmetric linear relation, and the graph, $\mathfrak{G}(B^*)$ of B^* is the adjoint relation to $\mathfrak{G}(B)$.

In this paper we will be considering closed symmetric linear transformations B with deficiency indices (n, n) , which are not necessarily densely defined. If this is the case then this means that B does not have a uniquely defined adjoint operator, and it will be convenient to identify B with its graph $\mathfrak{G}(B)$:

$$\mathfrak{G}(B) := \{(f, Bf) \mid f \in \text{Dom}(B)\},$$

in which case

$$\mathfrak{G}(B)^* = \{(g_1, g_2) \mid \langle f, g_2 \rangle = \langle Bf, g_1 \rangle \quad \forall f \in \text{Dom}(B)\}$$

is a closed linear relation but not the graph of a linear operator. Indeed, observe that if $g \perp \text{Dom}(B)$ then by equation (3.1), $(0, g) \in \mathfrak{G}(B)^*$ since

$$\langle f, g \rangle = \langle Bf, 0 \rangle,$$

for every $(f, Bf) \in \mathfrak{G}(B)$. For convenience we will simply write B^* for $\mathfrak{G}(B)^*$ in the case where B is not densely defined. Note that

$$B^*(0) := \{f \in \mathcal{H} \mid (0, f) \in \mathfrak{G}(B)^* = B^*\} = \overline{\text{Dom}(B)}^\perp.$$

One can show that if B has deficiency indices (n, n) that the co-dimension of $\text{Dom}(B)$ is at most n :

Lemma 3.1. *If $B \in \mathcal{S}_n(\mathcal{H})$, the orthogonal complement of $\text{Dom}(B)$ is at most n -dimensional.*

Proof. If $V = b(B)$ then $\text{Ker}(V)$ is n -dimensional, and $\text{Dom}(B) = (1 - V)\text{Ker}(V)^\perp$. If $f \perp \text{Dom}(B)$, then

$$0 = \langle f, (1 - V)\text{Ker}(V)^\perp \rangle = \langle (1 - V^*)f, \text{Ker}(V)^\perp \rangle,$$

and so $(1 - V^*)f \in \text{Ker}(V)$ which is n -dimensional. Now $(1 - V^*)f \neq 0$ as then f would be an eigenfunction to eigenvalue 1 and V would not be simple. It follows that the dimension of $\text{Dom}(B)^\perp$ is at most n as otherwise we could find a $g \in \text{Dom}(B)^\perp$ such that $(1 - V^*)g = 0$. \square

For $z \in \mathbb{C}$ define

$$(B^* - z) := \{(f, g - zf) \mid (f, g) \in B^*\},$$

and

$$\text{Ker}(B^* - z) := \{f \in \mathcal{H} \mid (f, 0) \in (B^* - z)\}.$$

Then, as in the case of densely defined B , it follows that

$$\text{Ker}(B^* - z) = \text{Ran}(B - \bar{z})^\perp,$$

so that

$$\mathcal{H} = \text{Ran}(B - \bar{z}) \oplus \text{Ker}(B^* - z),$$

for any $z \in \mathbb{C} \setminus \mathbb{R}$.

If B is a symmetric linear transformation then one can show, whether or not B is densely defined, that

$$\dim(\text{Ker}(B^* - z)) \text{ is constant for } z \in \mathbb{C}_\pm,$$

so that one can define $n_\pm = \dim(\text{Ker}(B^* - z))$ for $z \in \mathbb{C}_\pm$. For lack of a reference, here is an elementary proof of this fact.

Proposition 3.2. *Let B be a symmetric linear transformation in a separable Hilbert space \mathcal{H} . Then $\dim(\text{Ker}(B^* - z))$ is constant in \mathbb{C}_+ and in \mathbb{C}_- .*

Proof. Given $w \in \mathbb{C} \setminus \mathbb{R}$ let $P_w :=$ projection onto $\text{Ker}(B^* - w) = \text{Ran}(B - \bar{w})^\perp$, and let $Q_w :=$ projection onto $\text{Ran}(B - w)$ so that $Q_w = 1 - P_{\bar{w}}$.

Now fix $w \in \mathbb{C} \setminus \mathbb{R}$. Choose any $f \in Q_w \mathcal{H}$ of unit norm, $\|f\| = 1$. Since $f \in \text{Ran}(B - w)$, we have that $f = (B - w)g$ for some $g \in \text{Dom}(B)$. Now $B - w$ is bounded below, an easy calculation shows that for any $g \in \text{Dom}(B)$:

$$\|(B - w)g\|^2 = \|(B - \text{Re}(w))g\|^2 + |\text{Im}(w)|^2 \|g\|^2 \geq |\text{Im}(w)|^2 \|g\|^2.$$

Hence

$$\|g\| \leq \frac{\|(B - w)g\|}{|\text{Im}(w)|} = \frac{\|f\|}{|\text{Im}(w)|} = \frac{1}{|\text{Im}(w)|}.$$

Now choose z in the same half-plane as w and consider:

$$\begin{aligned} Q_z Q_w f &= Q_z f = Q_z (B - w)g = Q_z ((B - z)g + (z - w)g) \\ &= (B - z)g + (z - w)Q_z g. \end{aligned}$$

It follows that

$$\begin{aligned} (Q_w - Q_z Q_w) f &= (B - w)g - (B - z)g - (z - w)Q_z g = (z - w)(1 - Q_z)g \\ &= (z - w)P_{\bar{z}} g. \end{aligned}$$

This implies that

$$\|(Q_w - Q_z Q_w) f\| \leq |z - w| \|g\| \leq \frac{|z - w|}{|\text{Im}(w)|}.$$

Since f was an arbitrary norm one vector in $Q_w\mathcal{H}$ we conclude that

$$\|Q_w - Q_z Q_w\| \leq \frac{|z - w|}{|\operatorname{Im}(w)|}.$$

Taking adjoints it follows that we also have

$$\|Q_w - Q_w Q_z\| \leq \frac{|z - w|}{|\operatorname{Im}(w)|}.$$

Now

$$\begin{aligned} \|Q_w - Q_z\| &= \|Q_w - Q_w Q_z + Q_w Q_z - Q_z\| \\ &\leq \|Q_w - Q_w Q_z\| + \|Q_z - Q_w Q_z\| \\ &\leq \frac{|z - w|}{|\operatorname{Im}(w)|} + \frac{|z - w|}{|\operatorname{Im}(z)|}. \end{aligned}$$

For fixed $w \in \mathbb{C}_+$ or \mathbb{C}_- , this is less than one for all z in a small enough neighbourhood of w .

It follows that for z close enough to w we have

$$\|P_{\bar{w}} - P_{\bar{z}}\| = \|(1 - Q_w) - (1 - Q_z)\| = \|Q_w - Q_z\| < 1,$$

so that by [1, Section 34] $P_{\bar{z}}\mathcal{H}$ and $P_{\bar{w}}\mathcal{H}$ have the same dimension. It follows that the dimension of $P_z\mathcal{H} = \operatorname{Ker}(B^* - z) = \operatorname{Ran}(B - \bar{z})^\perp$ is constant for $z \in \mathbb{C}_+$, and for $z \in \mathbb{C}_-$. \square

4. HERGLOTZ SPACES

In this section we will show that any $B \in \mathcal{S}_n$ is unitarily equivalent to the operator of multiplication by z in a certain space of analytic functions called a Herglotz space. Assume that $n < \infty$.

4.1. Herglotz Functions. It will be convenient to begin with a brief review of the Nevanlinna-Herglotz representation theory of Herglotz functions on both the unit disk \mathbb{D} and the upper half-plane \mathbb{C}_+ . Let g be a $\mathbb{C}^{n \times n}$ -valued Herglotz function on \mathbb{D} , *i.e.* an analytic function with non-negative real part. Here $\mathbb{C}^{n \times n}$ is our notation for the $n \times n$ matrices over \mathbb{C} . Then by the Herglotz representation theorem there is a unique positive Borel $\mathbb{C}^{n \times n}$ -valued measure on the unit circle \mathbb{T} such that

$$\operatorname{Re}(g(z)) = \int_{\mathbb{T}} \operatorname{Re} \left(\frac{\alpha + z}{\alpha - z} \right) \sigma(d\alpha).$$

The measure σ determines the Herglotz function g up to an imaginary constant so that

$$g(z) = ib + \int_{\mathbb{T}} \frac{\alpha + z}{\alpha - z} \sigma(d\alpha).$$

We will always impose the normalization condition that $b = 0$ in this paper. Observe that this means that σ is a probability measure, *i.e.* σ is unital, $\sigma(\mathbb{T}) = \mathbb{1}$, if and only if $g(0) = 0$. We will also extend g to a function on $\mathbb{C} \setminus \mathbb{T}$ using the convention that

$$g(1/\bar{z})^* = -g(z).$$

Now let $G := g \circ b$ be the corresponding matrix-valued Herglotz function on \mathbb{C}_+ (G has non-negative real part in \mathbb{C}_+). Setting $w := b^{-1}(z)$ and $t = b^{-1}(\alpha)$, we obtain that

$$G(w) = -i\sigma(\{1\})w + \int_{-\infty}^{\infty} \frac{wt+1}{i(t-w)}(\sigma \circ b)(dt).$$

The convention that $g(1/\bar{z})^* = -g(z)$ implies that $G(\bar{w})^* = -G(w)$ and this extends G to a function on $\mathbb{C} \setminus \mathbb{R}$. Again, we have that σ is unital if and only if $g(0) = \mathbb{1}$ which happens if and only if $G(i) = \mathbb{1}$.

Now the Herglotz theorem on the upper half-plane states that

$$\operatorname{Re}(G(w)) = cy + \int_{-\infty}^{\infty} P_w(t)\Sigma(dt),$$

for unique Borel measure Σ obeying

$$\int_{-\infty}^{\infty} \frac{\Sigma(dt)}{1+t^2} < \infty,$$

and positive constant matrix $c \geq 0$ where $y = \operatorname{Im}(w)$ and

$$P_w(t) = \operatorname{Re}\left(\frac{1}{i\pi} \frac{1}{t-w}\right).$$

It will be convenient to determine the relationship between the Herglotz measure σ of g and Σ of $G := g \circ b$. As above we let

$$z(w) = \frac{w-i}{w+i} = b(w) \quad \text{and} \quad w(z) = i\frac{1+z}{1-z} = b^{-1}(z).$$

The function $g := G \circ b^{-1}$ obeys

$$\operatorname{Re}(g(z)) = \int_{\mathbb{T}} p_z(\alpha)\sigma(d\alpha),$$

where

$$p_z(\alpha) = \operatorname{Re}\left(\frac{\alpha+z}{\alpha-z}\right),$$

is the Poisson kernel on the disk. We can write

$$\operatorname{Re}(g(z)) = p_z(1)\sigma(\{1\}) + \int_{\mathbb{T} \setminus \{1\}} p_z(\alpha)\sigma(d\alpha).$$

Now for $\alpha \in \mathbb{T} \setminus \{1\}$ we can let $\alpha = z(t)$ for $t \in \mathbb{R}$ to write

$$\operatorname{Re}(G(w)) = \operatorname{Re}(g(z(w))) = p_{z(w)}(1)\sigma(\{1\}) + \int_{-\infty}^{\infty} p_{z(w)}(z(t))\tilde{\sigma}(dt),$$

where $\tilde{\sigma}$ is the measure on \mathbb{R} defined by $\tilde{\sigma}(\Omega) := \sigma(z(\Omega)) = (\sigma \circ b)(\Omega)$, so that $z(\Omega) = b(\Omega) \in \mathbb{T} \setminus \{1\}$.

A bit of algebra shows that

$$p_z(1) = \frac{1-|z|^2}{|1-z|^2},$$

and that if $w = x + iy \in \mathbb{C}_+$, then

$$p_{z(w)}(1) = y.$$

Some more algebra shows that

$$P_w(t) = \frac{1}{2\pi i} \frac{w - \bar{w}}{|t-w|^2},$$

while

$$p_{z(w)}(z(t)) = \pi(1+t^2)P_w(t).$$

We conclude that

$$\operatorname{Re}(G(w)) = \operatorname{Re}(g(z(w))) = y\sigma(\{1\}) + \int_{-\infty}^{\infty} P_w(t)\pi(1+t^2)\tilde{\sigma}(dt).$$

Finally this shows how the measures $\tilde{\sigma}$ and Σ are related:

$$\Sigma(\Omega) = \int_{\Omega} \pi(1+t^2)(\sigma \circ b)(dt). \quad (4.1)$$

Now let Θ be an arbitrary contractive $n \times n$ matrix-valued analytic function on \mathbb{C}_+ . Then

$$G_{\Theta} := \frac{1+\Theta}{1-\Theta},$$

is a Herglotz function on \mathbb{C}_+ .

There is a bijective correspondence between $\mathbb{C}^{n \times n}$ -valued Herglotz functions G on $\mathbb{C} \setminus \mathbb{R}$ and $\mathbb{C}^{n \times n}$ -valued contractive analytic functions Θ on \mathbb{C}_+ defined by

$$\Theta \mapsto G_{\Theta} := \frac{1+\Theta}{1-\Theta} \quad \text{and} \quad G \mapsto \Theta_G := \frac{G-1}{G+1}.$$

The Nevanlinna-Herglotz representation theory can also be used to define a bijective correspondence between $\mathbb{C}^{n \times n}$ -valued Herglotz functions on \mathbb{C}^+ and a large class of $\mathbb{C}^{n \times n}$ -positive matrix-valued measures on \mathbb{R} . Namely if g is a Herglotz function on the unit disk which obeys the normalization condition of the previous section (no non-zero constant imaginary part), then as discussed above it is uniquely determined by a regular, positive $\mathbb{C}^{n \times n}$ -valued Borel measure on the unit circle \mathbb{T} by the formula:

$$g(z) = \int_{\mathbb{T}} \frac{\alpha+z}{\alpha-z} \sigma(d\alpha). \quad (4.2)$$

It follows that the Herglotz function $G := g \circ b$ on \mathbb{C}_+ is uniquely determined by the Herglotz measure Σ and the value of $\sigma(\{1\})$ by the formula

$$\begin{aligned} G(z) &= -i\sigma(\{1\})z + \int_{-\infty}^{\infty} \frac{zt+1}{i(t-z)} (\sigma \circ b)(dt) \\ &= -i\sigma(\{1\})z + \frac{1}{i\pi} \int_{-\infty}^{\infty} \frac{zt+1}{(t-z)} \frac{1}{1+t^2} \Sigma(dt). \end{aligned} \quad (4.3)$$

Conversely given any non-negative matrix $P \in \mathbb{C}^{n \times n}$ and positive $\mathbb{C}^{n \times n}$ matrix-valued Borel measure on \mathbb{R} that obeys the condition:

$$\left(\int_{-\infty}^{\infty} \frac{1}{1+t^2} \Sigma(dt) \vec{v}, \vec{w} \right)_{\mathbb{C}^n} < \infty, \quad (4.4)$$

for any $\vec{v}, \vec{w} \in \mathbb{C}^n$, there is a unique Herglotz function G on \mathbb{C}_+ that obeys equation (4.3), or equivalently obeys:

$$\operatorname{Re}(G(z)) = P \operatorname{Im}(z) + \int_{-\infty}^{\infty} \operatorname{Re} \left(\frac{1}{i\pi} \frac{1}{t-z} \right) \Sigma(dt).$$

It follows that there is a bijective correspondence between Herglotz functions G on \mathbb{C}_+ and such pairs (P, Σ) , where $P \in \mathbb{C}^{n \times n}$ is positive and Σ is a positive $\mathbb{C}^{n \times n}$ valued measure obeying the condition (4.4). This in turn implies there is a bijective correspondence between contractive analytic functions

Θ on \mathbb{C}_+ and such pairs (P, Σ) . Given Θ we will call the corresponding Σ the Herglotz measure of Θ and we will usually denote this by Σ_Θ . Similarly σ_θ will denote the Herglotz measure of $\theta := \Theta \circ b^{-1}$. Note that since we assume any Herglotz function g_θ obeys our normalization condition (no non-zero imaginary constant part), it follows that σ_θ is unital if and only if $g_\theta(0) = \mathbb{1} = G_\Theta(\mathbb{1})$ which happens if and only if $\theta(0) = 0 = \Theta(i)$.

4.2. Herglotz spaces. Let Θ be a $\mathbb{C}^{n \times n}$ -valued contractive analytic function on \mathbb{C}_+ . The Herglotz space, $\mathcal{L}(\Theta)$ is the abstract reproducing kernel space of analytic \mathbb{C}^n -valued functions on $\mathbb{C} \setminus \mathbb{R}$ with reproducing kernel

$$K_w^\Theta(z) := \frac{i}{\pi} \frac{G_\Theta(z) + G_\Theta(w)^*}{z - \bar{w}}.$$

Namely given any $\vec{v} \in \mathbb{C}^n$ and $f \in \mathcal{L}(\Theta)$ and $w \in \mathbb{C} \setminus \mathbb{R}$, we have that $K_w \vec{v} \in \mathcal{L}(\Theta)$ where $K_w \vec{v}(z) := K_w(z) \vec{v}$ and,

$$(f(z), \vec{v})_{\mathbb{C}^n} = \langle f, K_z^\Theta \vec{v} \rangle_\Theta.$$

As shown in [4], if Θ is a Livsic characteristic function so that $\Theta(i) = 0$, and the symmetric linear transformation B with characteristic function Θ is densely defined then one can define a closed simple symmetric linear operator $\mathfrak{Z}_\Theta \in \mathcal{S}_n(\mathcal{L}(\Theta))$ with domain

$$\text{Dom}(\mathfrak{Z}_\Theta) = \{f \in \mathcal{L}(\Theta) \mid zf \in \mathcal{L}(\Theta)\},$$

by

$$(\mathfrak{Z}_\Theta f)(z) := zf(z); \quad f \in \text{Dom}(\mathfrak{Z}_\Theta),$$

see [4, Theorem 6.3]. Since we do not assume that all of our symmetric linear transformations are densely defined, we will need to extend this slightly:

Lemma 4.3. *Let Θ be a contractive analytic $\mathbb{C}^{n \times n}$ -valued function on \mathbb{C}_+ . The linear transformation \mathfrak{Z}_Θ defined on the domain*

$$\text{Dom}(\mathfrak{Z}_\Theta) := \{F \in L(\Theta) \mid zF(z) \in L(\Theta)\},$$

by

$$(\mathfrak{Z}_\Theta F)(z) = zF(z), \quad F \in \text{Dom}(\mathfrak{Z}_\Theta)$$

belongs to $\mathcal{S}_n(L(\Theta))$.

The proof of this lemma follows from the vector-valued version of [12, Theorem 5], see also [13]. In particular we use the identity

$$(\bar{w} - w) \left\langle \frac{F - F(w)}{z - w}, \frac{G - G(w)}{z - w} \right\rangle_\Theta = \left\langle F, \frac{G - G(w)}{z - w} \right\rangle_\Theta - \left\langle \frac{F - F(w)}{z - w}, G \right\rangle_\Theta,$$

valid for all $F, G \in L(\Theta)$ proven in [12, Theorem 5] for the case $n = 1$, and easily verified to also hold for the vector-valued case.

Proof. Let $S_{\pm i} := \{F \in L(\Theta) \mid F(\pm i) = 0\}$. By de Branges' results on Herglotz spaces, if $F \in S_{-i}$ then

$$(VF)(z) := \frac{z - i}{z + i} F(z) = b(z)F(z) \in L(\Theta),$$

so that the linear transformation V which acts as multiplication by $b(z)$ obeys $V : S_{-i} \rightarrow S_i$. We can show that V is in fact an isometry: if $F \in S_{-i}$ then

$$\begin{aligned} \langle VF, VF \rangle_{\Theta} &= \left\langle F - \frac{2i}{z+i}F, F - \frac{2i}{z+i}F \right\rangle_{\Theta} \\ &= \langle F, F \rangle_{\Theta} - 2i \left(\left\langle \frac{1}{z+i}F, F \right\rangle_{\Theta} - \left\langle F, \frac{1}{z+i}F \right\rangle_{\Theta} \right) + \left\langle \frac{2i}{z+i}F, \frac{2i}{z+i}F \right\rangle_{\Theta} \\ &= \langle F, F \rangle_{\Theta}, \end{aligned}$$

using the identity stated before the proof.

It is not hard to verify that V is closed, and so $\mathfrak{Z}_{\Theta} := b^{-1}(V)$ is a well-defined closed symmetric linear transformation. The symmetric linear transformation \mathfrak{Z}_{Θ} has indices (n, n) since

$$\text{Ker}(\mathfrak{Z}_{\Theta}^* + i) = \text{Ker}(V) = \bigvee K_{-i}^{\Theta} \mathbb{C}^n,$$

and

$$\text{Ker}(\mathfrak{Z}_{\Theta}^* - i) = \text{Ran}(V)^{\perp} = \bigvee K_i^{\Theta} \mathbb{C}^n.$$

Similarly,

$$\text{Ker}(\mathfrak{Z}_{\Theta}^* - z) = \bigvee K_z^{\Theta} \mathbb{C}^n,$$

so that

$$\mathbf{L}(\Theta) = \bigvee_{z \in \mathbb{C} \setminus \mathbb{R}} \text{Ker}(\mathfrak{Z}_{\Theta}^* - z),$$

proving that \mathfrak{Z}_{Θ} is simple. It remains to check that the domain of \mathfrak{Z}_{Θ} is equal to

$$\mathfrak{D}_{\Theta} := \{F \in \mathbf{L}(\Theta) \mid zF(z) \in \mathbf{L}(\Theta)\}.$$

Clearly $\text{Dom}(\mathfrak{Z}_{\Theta}) \subset \mathfrak{D}_{\Theta}$, and conversely if $F \in \mathfrak{D}_{\Theta}$ then $G(z) = (z+i)F(z) \in S_{-i} = \text{Ker}(V)^{\perp}$, and so by definition $(1-V)G \in \text{Dom}(\mathfrak{Z}_{\Theta})$, and

$$(1-V)G(z) = (z+i)F(z) - (z-i)F(z) = 2iF(z).$$

This proves that $F \in \text{Dom}(\mathfrak{Z}_{\Theta})$ so that $\mathfrak{D}_{\Theta} = \text{Dom}(\mathfrak{Z}_{\Theta})$. □

Lemma 4.4. *Let Θ be a contractive analytic function as above. The Livsic characteristic function of \mathfrak{Z}_{Θ} is a Frostman shift of Θ :*

$$\Theta_{\mathfrak{Z}_{\Theta}} = (1 - \Theta(i)^*)(1 - \Theta\Theta(i)^*)^{-1}(\Theta - \Theta(i))(1 - \Theta(i))^{-1}.$$

Proof. This is a straightforward calculation using the definition of the characteristic function (equations (2.6), (2.7) and (2.8)) and the reproducing kernel

$$K_w(z) = \frac{i}{\pi} \frac{G_{\Theta}(z) + G_{\Theta}(w)^*}{z - \overline{w}},$$

for $\mathcal{L}(\Theta)$. Let $\{e_j\}$ be the standard orthonormal basis of \mathbb{C}^n . We can choose

$$u_j = K_{-i}K_{-i}(-i)^{-1/2}e_j, \quad v_j = K_iK_i(i)^{-1/2}e_j \quad \text{and} \quad w_j(z) := K_{\overline{z}}e_j.$$

With this choice of bases, one obtains

$$A(z) = [\langle K_{\overline{z}}e_j, K_iK_i(i)^{-1/2}e_k \rangle] = K_i(i)^{-1/2}K_{\overline{z}}(i) \quad \text{and} \quad B(z) = K_{-i}(-i)^{-1/2}K_{\overline{z}}(-i).$$

Recall here that

$$\Theta_{\mathfrak{Z}_\Theta}(z) = b(z)B(z)^{-1}A(z).$$

Now observe that

$$K_i(i) = \frac{i}{\pi} \frac{G_\Theta(i) + G_\Theta(i)^*}{2i}.$$

Using that $G_\Theta(\bar{z})^* = -G_\Theta(z)$ for the Herglotz function G_Θ , we also obtain that

$$K_{-i}(-i) = \frac{i}{\pi} \frac{G_\Theta(-i) + G_\Theta(-i)^*}{-2i} = \frac{i}{\pi} \frac{-G_\Theta(i)^* - G_\Theta(i)}{-2i} = K_i(i).$$

It follows that

$$\Theta(z) := \Theta_{\mathfrak{Z}_\Theta}(z) = b(z)B(z)^{-1}A(z) = b(z)K_{\bar{z}}(-i)^{-1}K_{\bar{z}}(i).$$

Substituting in our expression for the reproducing kernel $K_w(z)$ yields

$$\begin{aligned} \Theta(z) &= b(z) \left(\frac{i}{\pi} \frac{G(-i) + G(\bar{z})^*}{-i - z} \right)^{-1} \left(\frac{i}{\pi} \frac{G(i) + G(\bar{z})^*}{i - z} \right) \\ &= (G(-i) + G(\bar{z})^*)^{-1} (G(i) + G(\bar{z})^*) \\ &= (-G(i)^* - G(z))^{-1} (G(i) - G(z)) \\ &= (G(i)^* + G(z))^{-1} (G(i) - G(z)). \quad (\text{ignore the factor of } -1) \end{aligned}$$

We can ignore the factor of -1 since $\Theta(z)$ is defined only up to conjugation by fixed unitaries.

Now straightforward algebra shows that

$$G(z) - G(i) = 2(1 - \Theta(z))^{-1}(\Theta(z) - \Theta(i)(1 - \Theta(i))^{-1}),$$

while

$$G(i)^* + G(z) = 2(1 - \Theta(z))^{-1}(1 - \Theta(z)\Theta(i)^*)(1 - \Theta(i)^*)^{-1}.$$

Putting these two formulas together yields the Frostman shift formula. \square

In particular if $\Theta(i) = 0$ then Θ is equal to the Livsic characteristic function of \mathfrak{Z}_Θ , and Theorem 2.1 allows us to conclude:

Corollary 4.5. *If $B \in \mathcal{S}$ has characteristic function Θ then $B \cong \mathfrak{Z}_\Theta$.*

The following example of symmetric extensions of a symmetric operator B with Θ_B inner will be important:

Example 4.6. Let Θ, Φ be $\mathbb{C}^{n \times n}$ -valued inner functions on \mathbb{C}_+ such that $\Theta \leq \Phi$. In this case $\Theta^{-1}\Phi$ is also an inner function.

Given any inner function Θ one can define a symmetric linear transformation Z_Θ acting in K_Θ^2 by:

$$\text{Dom}(Z_\Theta) := \{f \in K_\Theta^2 \mid zf(z) \in K_\Theta^2\},$$

and

$$Z_\Theta f(z) := zf(z), \quad f \in \text{Dom}(Z_\Theta),$$

see for example [3, 4]. It is straightforward to show that the characteristic function of Z_Θ is the Frostman shift of Θ as above so that by Livsic's theorem $Z_\Theta \simeq \mathfrak{Z}_\Theta$.

It follows that since $K_\Theta^2 \subset K_\Phi^2$ that $\text{Dom}(Z_\Theta) \subset \text{Dom}(Z_\Phi)$ and that $Z_\Theta \subset Z_\Phi$ so that $Z_\Theta \lesssim Z_\Phi$. Moreover given any $A \in \text{Ext}(Z_\Phi)$, then the restriction A' of A to its smallest invariant subspace containing K_Θ^2 belongs to $\text{Ext}(Z_\Theta)$.

This can be generalized further: Suppose that Φ is an arbitrary contractive analytic function such that $\Phi \geq \Theta$ where Θ is inner. Then by [14, II-6], K_Θ^2 is contained isometrically in the deBranges-Rovnyak space K_Φ^2 , $K_\Theta^2 \subset K_\Phi^2$. Moreover [4, Theorem 7.1] shows that multiplication by $V(z) := \frac{2}{1-\Phi(z)}$ is an isometry from K_Φ^2 into $\mathcal{L}(\Phi)$. Hence $V : K_\Theta^2 \rightarrow \mathcal{L}(\Phi)$, the operator of multiplication by $V(z)$ is an isometry of K_Θ^2 into $\mathcal{L}(\Phi)$, and by the definition of $\text{Dom}(Z_\Theta)$, and the definition of $\text{Dom}(\mathfrak{Z}_\Phi)$ in Lemma 4.3, it follows that $V\text{Dom}(Z_\Theta) \subset \text{Dom}(\mathfrak{Z}_\Phi)$ and that $VZ_\Theta V^* \subset \mathfrak{Z}_\Phi$ so that $Z_\Theta \lesssim \mathfrak{Z}_\Phi$. Since $\mathfrak{Z}_\Theta \cong Z_\Theta$, this also shows that $\mathfrak{Z}_\Theta \lesssim \mathfrak{Z}_\Phi$ whenever Θ is inner, Φ is contractive and $\Theta \leq \Phi$. Again the restriction of any $A \in \text{Ext}(\mathfrak{Z}_\Phi)$ to its smallest invariant subspace containing VK_Θ^2 belongs to $\text{Ext}_U(Z_\Theta)$. Here recall that given $B \in \mathcal{S}$, $\text{Ext}_U(B)$ is the set of all self-adjoint linear transformations A such that $A \in \text{Ext}(UBU^*)$ for some isometry $U : \mathcal{H} \rightarrow \mathcal{K}$.

We can also construct examples of symmetric $B_1 \in \mathcal{S}_n(\mathcal{H}_1)$ and $B_2 \in \mathcal{S}_m(\mathcal{H}_2)$ such that $B_1 \lesssim B_2$ where $n \neq m$: Suppose that $\Phi := \Theta\Gamma$ where Φ, Θ, Γ are all scalar-valued inner functions on \mathbb{C}_+ . Let

$$\Lambda := \begin{pmatrix} \Theta & 0 \\ 0 & \Gamma \end{pmatrix}.$$

Then Λ is a 2×2 matrix-valued inner function, and note that Z_Λ has indices $(2, 2)$, and that there is a natural unitary map W from $K_\Lambda^2 = K_\Theta^2 \oplus K_\Gamma^2$ onto $K_\Phi^2 = K_\Theta^2 \oplus \Theta K_\Gamma^2$. Namely

$$W(f \oplus g) := f + \Theta g,$$

so that if we view elements of K_Λ^2 as column vectors then W acts as multiplication by the 1×2 matrix function

$$W(z) = (1, \Theta(z)).$$

It follows that $Z_\Lambda \lesssim Z_\Phi$, where Z_Λ has indices $(2, 2)$ and Z_Φ has indices $(1, 1)$.

Theorem 4.7. *If $B_1, B_2 \in \mathcal{S}$ with characteristic functions Θ_1, Θ_2 , the characteristic function Θ_1 is inner and $\Theta_1 \leq \Theta_2$ then $B_1 \lesssim B_2$.*

Proof. By Corollary 4.5, $B_j \simeq \mathfrak{Z}_{\Theta_j}$. As discussed in the above example if Θ_1 is inner and $\Theta_1 \leq \Theta_2$ then $\mathfrak{Z}_{\Theta_1} \lesssim \mathfrak{Z}_{\Theta_2}$ so that $B_1 \lesssim B_2$. \square

Given any $B \in \mathcal{S}_1(\mathcal{H})$, it is well known that there is a conjugation C_B which commutes with B , i.e. $C_B : \text{Dom}(B) \rightarrow \text{Dom}(B)$ and $C_B B = B C_B$. Recall here that a conjugation is an anti-linear, idempotent onto isometry [5, Theorem 7.1]. It will be useful for us to extend this construction to the case of arbitrary $B \in \mathcal{S}$. We say that C is a conjugation intertwining $B_1 \in \mathcal{S}_n(\mathcal{H}_1)$ and $B_2 \in \mathcal{S}_m(\mathcal{H}_2)$ provided that $C B_1 = B_2 C$, and C is an anti-linear and onto isometry.

Proposition 4.8. *Let Θ be a contractive $\mathbb{C}^{n \times n}$ -valued analytic function in \mathbb{C}_+ , $n \in \mathbb{N}$. The map $C_\Theta : L(\Theta) \rightarrow L(\Theta^T)$, defined by $C_\Theta F(z) = F^\dagger(z) := \overline{F(\bar{z})}$ is a conjugation intertwining \mathfrak{Z}_Θ and \mathfrak{Z}_{Θ^T} , and $C_\Theta^* = C_{\Theta^T}$.*

In the above T denotes matrix transpose and for a vector $F(z)$, $\overline{F(z)}$ denotes the vector obtained by taking the complex conjugate of each component in the fixed canonical basis of \mathbb{C}^n .

Proof. Let $\{e_k\}$ denote the canonical orthonormal basis of \mathbb{C}^n . Let $C : \mathbb{C}^n \rightarrow \mathbb{C}^n$ denote the conjugation defined by entrywise complex conjugation: if $\vec{v} = \sum c_i e_i$ for $c_i \in \mathbb{C}$, then $C\vec{v} := \sum \bar{c}_i e_i$. Given any matrix $A \in \mathbb{C}^{n \times n}$, with entries $A = [a_{ij}]$, it is easy to check that $CAC = [\overline{a_{ij}}] = (A^*)^T = (A^T)^*$. By definition, given $F \in \mathbf{L}(\Theta)$, we have that

$$(C_\Theta F)(z) = C(F(\bar{z})).$$

The closed linear span of the evaluation vectors $K_w^\Theta \vec{v}$ for $w \in \mathbb{C} \setminus \mathbb{R}$, $\vec{v} \in \mathbb{C}^n$ is dense in $\mathbf{L}(\Theta)$. The action of C_Θ on such functions is

$$\begin{aligned} (C_\Theta K_w^\Theta)(z) \vec{v} &= C K_w^\Theta(\bar{z}) \vec{v} = C K_w^\Theta(\bar{z}) C C \vec{v} \\ &= (K_w^\Theta(\bar{z})^T)^* C \vec{v}. \end{aligned}$$

Now

$$\begin{aligned} K_w^\Theta(\bar{z})^T &= \left(\frac{i}{\pi} \frac{G_\Theta(\bar{z}) + G_\Theta(w)^*}{\bar{z} - \bar{w}} \right)^T \\ &= \frac{i}{\pi} \frac{G_{\Theta^T}(\bar{z}) + G_{\Theta^T}(w)^*}{\bar{z} - \bar{w}}, \end{aligned}$$

since $G_\Theta = \frac{1+\Theta}{1-\Theta}$ so that $G_\Theta^T = G_{\Theta^T}$. It follows that

$$\begin{aligned} C K_w^\Theta(\bar{z}) C &= (K_w^\Theta(\bar{z})^T)^* \\ &= \frac{-i}{\pi} \frac{G_{\Theta^T}(\bar{z})^* + G_{\Theta^T}(w)}{z - w} \\ &= \frac{i}{\pi} \frac{G_{\Theta^T}(z) + G_{\Theta^T}(\bar{w})^*}{z - w} = K_{\bar{w}}^{\Theta^T}(z). \end{aligned}$$

This proves that

$$C_\Theta K_w^\Theta \vec{v} = K_{\bar{w}}^{\Theta^T} C \vec{v} \in \mathbf{L}(\Theta^T),$$

and it follows from the density of the point evaluation vectors that $C_\Theta : \mathbf{L}(\Theta) \rightarrow \mathbf{L}(\Theta^T)$, and that it has dense range. It is clear by definition that C_Θ is anti-linear. To see that it is an (anti-linear) isometry note that

$$\begin{aligned} \langle C_\Theta K_w^\Theta \vec{v}, C_\Theta K_z^\Theta \vec{w} \rangle_\Theta &= \left\langle K_{\bar{w}}^{\Theta^T} C \vec{v}, K_{\bar{z}}^{\Theta^T} C \vec{w} \right\rangle_{\Theta^T} \\ &= \left(K_{\bar{w}}^{\Theta^T}(\bar{z}) C \vec{v}, C \vec{w} \right)_{\mathbb{C}^n} \\ &= (C K_w^\Theta(z) C C \vec{v}, C \vec{w}) \\ &= (\vec{w}, K_w^\Theta(z) \vec{v}) = \langle K_z^\Theta \vec{w}, K_w^\Theta \vec{v} \rangle_\Theta. \end{aligned}$$

Using the fact that linear combinations of such functions are dense in $\mathbf{L}(\Theta)$ and $\mathbf{L}(\Theta^T)$, we conclude that C_Θ is an isometry with dense range, and hence is onto. In other words, C_Θ is anti-unitary, so that $C_\Theta^* C_\Theta = \mathbb{1}$. As is easy to check:

$$C_{\Theta^T} C_\Theta K_w^\Theta \vec{v} = C_{\Theta^T} K_{\bar{w}}^{\Theta^T} C \vec{v} = K_w^\Theta C^2 \vec{v} = K_w^\Theta \vec{v},$$

and it follows that $C_\Theta^* = C_{\Theta^T}$.

Finally, since $\text{Dom}(\mathfrak{Z}_\Theta) := \{F \in \mathbf{L}(\Theta) \mid zF \in \mathbf{L}(\Theta)\}$, and similarly for $\mathfrak{Z}_{\Theta^\tau}$, $C_\Theta \text{Dom}(\mathfrak{Z}_\Theta) = \text{Dom}(\mathfrak{Z}_{\Theta^\tau})$. Indeed, if $F \in \text{Dom}(\mathfrak{Z}_\Theta)$, then

$$C_\Theta zF(z) = C(\bar{z}F(\bar{z})) = z(C_\Theta F)(z),$$

so that $C_\Theta F \in \text{Dom}(\mathfrak{Z}_{\Theta^\tau})$, and conversely given any $G \in \text{Dom}(\mathfrak{Z}_{\Theta^\tau})$, $C_{\Theta^\tau} G \in \text{Dom}(\mathfrak{Z}_\Theta)$, and $C_\Theta C_{\Theta^\tau} G = G$, showing that $C_\Theta \text{Dom}(\mathfrak{Z}_\Theta) = \text{Dom}(\mathfrak{Z}_{\Theta^\tau})$. The above arguments also show that for any $F \in \text{Dom}(\mathfrak{Z}_\Theta)$,

$$C_\Theta \mathfrak{Z}_\Theta F = \mathfrak{Z}_{\Theta^\tau} C_\Theta F,$$

completing the proof. \square

Corollary 4.9. *Suppose that $B \in \mathcal{S}_n(\mathcal{H})$ has characteristic function Θ_B . Let $B_T \in \mathcal{S}_n(\mathcal{H}_T)$ have characteristic function $\Theta_{B_T}^T$. Then there are conjugations $C_B : \mathcal{H} \rightarrow \mathcal{H}_T$, and $C_{B^\tau} = C_B^*$ such that $C_B B = B_T C_B$ and $C_{B^\tau} B_T = B C_{B^\tau}$.*

Note that any such conjugation C_B obeys $C_B \text{Ran}(B - z) = \text{Ran}(B_T - \bar{z})$, $C_B \text{Ker}(B^* - z) = \text{Ker}(B_T^* - \bar{z})$, and $C_B b(B) = b(B_T)^* C_B$.

Proof. We have $B \simeq \mathfrak{Z}_\Theta$ and $B_T \simeq \mathfrak{Z}_{\Theta^\tau}$. Composing the unitary operators effecting these equivalences with C_Θ yields C_B . \square

4.10. Measure spaces. Let Σ be any $\mathbb{C}^{n \times n}$ positive regular matrix-valued measure on \mathbb{R} which obeys the Herglotz condition:

$$\left(\int_{-\infty}^{\infty} \frac{1}{1+t^2} \Sigma(dt) \vec{v}, \vec{w} \right)_{\mathbb{C}^n} < \infty,$$

for any $\vec{v}, \vec{w} \in \mathbb{C}^n$. We define the measure space L_Σ^2 to be the space of all \mathbb{C}^n -valued functions on \mathbb{R} which are square-integrable with respect to Σ , i.e. $f \in L_\Sigma^2$ provided that

$$\int_{-\infty}^{\infty} (\Sigma(dt) f(t), f(t))_{\mathbb{C}^n} < \infty.$$

for any $z \in \mathbb{C} \setminus \mathbb{R}$, define the $\mathbb{C}^{n \times n}$ matrix function

$$\delta_z(t) := \frac{i}{\pi} \frac{1}{t - \bar{z}} \mathbb{1}_n.$$

Suppose that Θ is a contractive analytic function such that

$$\text{Re}(G_\Theta(z)) = P \text{Im}(z) + \int_{-\infty}^{\infty} \text{Re} \left(\frac{i}{\pi} \frac{1}{t - z} \right) \Sigma(dt).$$

The deBranges isometry

$$W_\Theta : L_\Sigma^2 \rightarrow \mathbf{L}(\Theta),$$

defined by

$$((W_\Theta h)(z), \vec{v})_{\mathbb{C}^n} := \left(\frac{1}{i\pi} \int_{-\infty}^{\infty} \frac{1}{\pi(t - \bar{z})} \Sigma(dt) h(t), \vec{v} \right) = \langle h, \delta_z \vec{v} \rangle_\Sigma,$$

where $\langle \cdot, \cdot \rangle_\Sigma$ denotes the inner product in L_Σ^2 is an isometry of $L_\Theta^2 := L_\Sigma^2$ into $\mathbf{L}(\Theta)$. The range of W_Θ is $\mathbf{L}(\Psi) \subset \mathbf{L}(\Theta)$ where

$$G_\Psi(z) = G_\Theta(z) + izP,$$

and the orthogonal complement of the range of W_Θ is the closed linear span of the constant functions $\bigvee P\mathbb{C}^n$. One can then check that the reproducing kernel for $L(\Theta)$ is given by the formula

$$(K_w^\Theta(z)\vec{v}, \vec{w})_{\mathbb{C}^n} = \left((\pi W \delta_w(z) + \frac{P}{\pi})\vec{v}, \vec{w} \right) = \langle \delta_w \vec{v}, \delta_z \vec{w} \rangle_\Sigma + \left(\frac{P}{\pi} \vec{v}, \vec{w} \right)_{\mathbb{C}^n} \quad (4.5)$$

Also notice that if $P = 0$ and Θ is a characteristic function so that $\Theta(i) = 0$, that this implies that $G_\Theta(i) = \mathbb{1}$ so that

$$\mathbb{1} = \int_{-\infty}^{\infty} \operatorname{Re} \left(\frac{1}{i\pi} \frac{1}{t-i} \right) \Sigma(dt) = \int_{-\infty}^{\infty} \frac{1}{1+t^2} \Sigma(dt),$$

and this implies that the vectors $\delta_i e_k$, $1 \leq k \leq n$ are an orthonormal set.

5. NON-CANONICAL REPRESENTATIONS OF SYMMETRIC OPERATORS

We are now sufficiently prepared to begin pursuing the main theory and results of this paper. For any $A \in \operatorname{Ext}(B)$ we can construct a representation of B as multiplication on a space of analytic functions on $\mathbb{C} \setminus \mathbb{R}$ as follows:

Let

$$\mathcal{K}_z := \mathcal{K} \ominus \operatorname{Ran}(B - \bar{z}) = (\mathcal{K} \ominus \mathcal{H}) \oplus \operatorname{Ker}(B^* - z).$$

For any $w, z \in \mathbb{C} \setminus \mathbb{R}$, if A is densely defined (so that $A = b^{-1}(U)$ and U does not have 1 as an eigenvalue) let

$$U_{w,z} := (A - w)(A - z)^{-1}. \quad (5.1)$$

If However $A = b^{-1}(U)P_U(\mathbb{T} \setminus \{1\})$ and U is a unitary extension of $V = b(B)$ which has 1 as an eigenvalue let

$$U_{w,z} := ((i - w) + U(i + w))((i - z) + U(i + z))^{-1}. \quad (5.2)$$

These two formulas coincide when U does not have 1 as an eigenvalue.

Then it is not difficult to verify as in [5, Section 1.2] that (regardless of whether A is densely defined or not) for any $w, z \in \mathbb{C} \setminus \mathbb{R}$, $U_{w,z}$ has the following properties:

- (1) $U_{w,z}$ is invertible.
- (2) $U_{w,z} : \mathcal{K}_w \rightarrow \mathcal{K}_z$ is a bijection.

Note that

$$P_{\mathcal{H}} U_{w,z} \operatorname{Ker}(B^* - w) \subset P_{\mathcal{H}} (\operatorname{Ker}(B^* - z) \oplus (\mathcal{K} \ominus \mathcal{H})) \subset \operatorname{Ker}(B^* - z).$$

Given any fixed $w \in \mathbb{C} \setminus \mathbb{R}$, let $J_w : \mathbb{C}^n \rightarrow \operatorname{Ker}(B^* - w)$ be a bounded isomorphism (a bounded linear map with bounded inverse). We can then define the map

$$\Gamma_A^w : \mathbb{C} \setminus \mathbb{R} \rightarrow \mathcal{B}(\mathbb{C}^n, \mathcal{H}),$$

by

$$\Gamma_A^w(z) := P_{\mathcal{H}} U_{w,\bar{z}} P_w J_w = P_{\mathcal{H}} (A - w)(A - \bar{z})^{-1} J_w, \quad (5.3)$$

(the last formula holds for the case where A is densely defined) where P_w projects onto $\operatorname{Ker}(B^* - w)$ and it follows that if $A \in \operatorname{Ext}(B)$ is actually a canonical element of $\operatorname{Ext}(B)$ that Γ_A is a *model* for B as defined in [4]. Namely, recall:

Definition 5.1. Given $B \in \mathcal{S}_n(\mathcal{H})$, let \mathcal{J} be a Hilbert space with $\dim(\mathcal{J}) = n$. A map $\Gamma : \mathbb{C} \setminus \mathbb{R} \rightarrow \mathcal{B}(\mathcal{J}, \mathcal{H})$, the space of bounded linear maps from \mathcal{J} to \mathcal{H} , is a *model* for B if Γ satisfies the following conditions:

$$\Gamma : \mathbb{C} \setminus \mathbb{R} \rightarrow \mathcal{B}(\mathcal{J}, \mathcal{H}) \text{ is co-analytic;} \quad (5.4)$$

$$\Gamma(\lambda) : \mathcal{J} \rightarrow \text{Ran}(B - \lambda I)^\perp \text{ is invertible for each } \lambda \in \mathbb{C} \setminus \mathbb{R}; \quad (5.5)$$

$$\Gamma(z)^* \Gamma(\lambda) : \mathcal{J} \rightarrow \mathcal{J} \text{ is invertible when } \lambda, z \in \mathbb{C}_+ \text{ and when } \lambda, z \in \mathbb{C}_-; \quad (5.6)$$

$$\bigvee_{\Im \lambda \neq 0} \text{Ran}(\Gamma(\lambda)) = \mathcal{H}, \quad (5.7)$$

where \bigvee denotes the closed linear span.

Recall that as shown in [4], any model Γ for $B \in \mathcal{S}_n(\mathcal{H})$ can be used to construct a reproducing kernel Hilbert space of analytic functions \mathcal{H}_Γ on $\mathbb{C} \setminus \mathbb{R}$ and a unitary $U_\Gamma : \mathcal{H} \rightarrow \mathcal{H}_\Gamma$ such that the image of B under this unitary transformation acts as multiplication by z .

Now if $A \in \text{Ext}(B)$ is non-canonical then Γ_A^w as defined in equation (5.3) does not necessarily satisfy the conditions of a model as defined in Definition 5.1. Despite this Γ_A^w has similar properties to a model and can still be used to construct a reproducing kernel Hilbert space of analytic functions \mathcal{H}_A on $\mathbb{C} \setminus \mathbb{R}$, and (at least in the case under consideration where Θ_B is inner) an isometry $U_A : \mathcal{H} \rightarrow \mathcal{H}_A$ such that $U_A B U_A^*$ again acts as multiplication by z in \mathcal{H}_A .

This motivates the definition of a non-canonical model which includes these generalized models Γ_A arising from non-canonical $A \in \text{Ext}(B)$:

Definition 5.2. Let \mathcal{J} be any n -dimensional Hilbert space and suppose that $B \in \mathcal{S}_n(\mathcal{H})$. If $\mathcal{B}(\mathcal{J}, \mathcal{H})$ is the space of bounded linear maps from \mathcal{J} to \mathcal{H} , we say that $\Gamma : \mathbb{C} \setminus \mathbb{R} \rightarrow \mathcal{B}(\mathcal{J}, \mathcal{H})$ is a *quasi-model* for $B \in \mathcal{S}_n(\mathcal{H})$ if Γ satisfies the following two conditions:

$$\Gamma : \mathbb{C} \setminus \mathbb{R} \rightarrow \mathcal{B}(\mathcal{J}, \mathcal{H}) \text{ is co-analytic;} \quad (5.8)$$

$$\Gamma(z) : \mathcal{J} \rightarrow \text{Ker}(B^* - \bar{z}). \quad (5.9)$$

Given a quasi-model Γ , we define

$$m_\pm := \max_{z \in \mathbb{C}_\pm} \dim(\text{Ker}(\Gamma(z))^\perp), \quad (5.10)$$

Γ is then said to have *rank* (m_-, m_+) , $0 \leq m_\pm \leq n$. The quasi-model Γ is said to have full rank if $m_+ = n = m_-$.

5.3. Basic properties of quasi-models.

Definition 5.4. Let Π_Γ^+ be the set of all points in \mathbb{C}_+ for which $\dim(\text{Ker}(\Gamma(z))^\perp) = m_+$, and define Π_Γ^- similarly. Let $\Sigma_\Gamma^\pm := \mathbb{C}_\pm \setminus \Pi_\Gamma^\pm$. We will also use the notation $\Pi_\Gamma = \Pi_\Gamma^+ \cup \Pi_\Gamma^-$ and $\Sigma_\Gamma = \Sigma_\Gamma^+ \cup \Sigma_\Gamma^-$.

We will now show that any quasi-model Γ of rank (n, n) has a property similar to the property (5.6) for a model.

Proposition 5.5. *If $B \in \mathcal{S}_n(\mathcal{H})$ and Γ is a quasi-model for B then $\Gamma(z)^* \Gamma(w)$ is a quasi-affinity on \mathcal{J} whenever $m_+ = n$ and $z, w \in \Pi_\Gamma^+$ or whenever $m_- = n$ and $z, w \in \Pi_\Gamma^-$.*

Remark 5.6. Note that in the case where $n < \infty$, which is the case we are primarily studying, when $\Gamma(z)^*\Gamma(w)$ is a quasi-affinity, it is acting between finite dimensional spaces and hence is in fact bounded and invertible. Also the reason this proposition is important is that we will shortly construct a reproducing kernel Hilbert space \mathcal{H}_Γ whose reproducing kernel is $K_w(z) = \Gamma^*(z)\Gamma(w)$, and it will be useful to know when this is invertible.

This proposition will be the consequence of the following:

Proposition 5.7. *For each $z \in \mathbb{C} \setminus \mathbb{R}$, let $\{\delta_k(z)\}_{k=1}^n$ be a basis for $\text{Ker}(B^* - z)$. Then the linear operator Y on $l^2(\mathbb{N})$ with entries*

$$Y(w, z) := [\langle \delta_j(w), \delta_k(z) \rangle]_{1 \leq j, k \leq n},$$

is a quasi-affinity for any $z, w \in \mathbb{C}_+$ or $z, w \in \mathbb{C}_-$, i.e. it is injective and has dense range (and hence an inverse which is potentially unbounded).

The proof of this proposition needs a little set up. Given a closed linear transformation T with domain $\text{Dom}(T) \subset \mathcal{H}$, a point $z \in \mathbb{C}$ is called a *regular* point of T if $T - z$ is bounded below on $\text{Dom}(T)$, i.e., $\|(T - z)f\| \geq c_z\|f\|$ for all $f \in \text{Dom}(T)$. Let Ω_T denote the set of regular points of T . If $B \in \mathcal{S}_n(\mathcal{H})$, then since B is symmetric we have that $\mathbb{C} \setminus \mathbb{R} \subset \Omega_B \subset \mathbb{C}$. The symmetric linear transformation B is called regular if $\Omega_B = \mathbb{C}$. For any $z \in \Omega_B$, let \mathfrak{G}_z be the closure of the linear relation: $\mathfrak{G}(B) \dot{+} \{(h_z, zh_z) \mid h_z \in \text{Ker}(B^* - z)\}$, and $\dot{+}$ denotes the non-orthogonal direct sum of linearly independent subspaces.

Lemma 5.8. *There is a closed linear operator B_z extending B such that $\mathfrak{G}(B_z) = \mathfrak{G}_z$.*

Proof. It suffices to prove that \mathfrak{G}_z is the graph of a densely defined closed linear operator.

Clearly $\mathfrak{G}(B_z) \subset B^*$. To prove that $\mathfrak{G}(B_z)$ is the graph of a linear transformation, we need to prove that the intersection of the multi-valued part of B^* with \mathfrak{G}_z is the zero element:

$$\{(0, g) \mid g \in B^*(0)\} \cap \mathfrak{G}_z = \{(0, 0)\},$$

where recall that $B^*(0) = \text{Dom}(B)^\perp$.

Suppose not, then we can find a sequence $(f_n) \subset \text{Dom}(B)$ and a sequence $h_n \in \text{Ker}(B^* - z)$ such that $(f_n + h_n, Bf_n + zh_n) \rightarrow (0, g)$ where $g \perp \text{Dom}(B)$. It follows that

$$(B - z)f_n = Bf_n + zh_n - z(f_n + h_n) \rightarrow g - 0 = g.$$

Since $\text{Ran}(B - z)$ is closed it follows that there is an $f \in \text{Dom}(B)$ such that

$$(B - z)f = g \perp \text{Dom}(B).$$

However this would then imply that

$$0 = \langle g, f \rangle = \langle (B - z)f, f \rangle = \langle Bf, f \rangle - z \langle f, f \rangle,$$

which is impossible as B is symmetric and $z \in \mathbb{C} \setminus \mathbb{R}$. This proves that \mathfrak{G}_z is the graph of a linear transformation B_z , it remains to prove that B_z is densely defined.

To prove that B_z is a linear operator, i.e. densely defined, suppose that $\phi \in \mathcal{H}$ is orthogonal to $\text{Dom}(B_z)$. Then $\phi \perp \text{Dom}(B)$ and $\phi \perp \text{Ker}(B^* - z)$. Hence $\phi \in \text{Ran}(B - \bar{z})$ and so $\phi = (B - \bar{z})f$

for some $f \in \text{Dom}(B)$. But ϕ is orthogonal to $\text{Dom}(B)$ as well so that

$$0 = \langle f, \phi \rangle = \langle f, (B - \bar{z})f \rangle,$$

showing that

$$\langle Bf, f \rangle = z \langle f, f \rangle,$$

which as before is impossible as B is symmetric. \square

Lemma 5.9. *Suppose that $z \in \mathbb{C} \setminus \mathbb{R}$. The spectrum of the operator B_z is contained in $\overline{\mathbb{C}_+}$ or $\overline{\mathbb{C}_-}$ when $z \in \mathbb{C}_+$ or \mathbb{C}_- , respectively.*

Since B_z is a closed linear operator, the proof is identical to that of [4, Lemma 2.6], and we omit it.

Proof. (of Proposition 5.7) Given a unit vector $\vec{c} \in \mathbb{C}^n$ (we take $\mathbb{C}^\infty := \ell^2(\mathbb{N})$), let

$$\Delta_{\vec{c}}(z) := \sum_k \overline{c_k} \delta_k(z).$$

Now observe that

$$Y(w, z)\vec{c} = (\langle \delta_j(w), \Delta_{\vec{c}}(z) \rangle)_{1 \leq j \leq n}.$$

Now if $Y(w, z)$ was not injective then there would be a $\vec{c} \in \mathbb{C}^n$ for which $Y\vec{c} = 0$, and hence $0 = \langle \delta_j(w), \Delta_{\vec{c}}(z) \rangle$ so that $\psi_z := \Delta_{\vec{c}}(z) \perp \text{Ker}(B^* - w)$ and hence $\psi_z \in \text{Ran}(B - \bar{w})$, $\psi_z = (B - \bar{w})f$ for some $f \in \text{Dom}(B)$. But then, since \bar{w} does not belong to the spectrum of B_z ,

$$(z - \bar{w})^{-1} \psi_z = (B_z - \bar{w})^{-1} \psi_z = f,$$

which shows that $\psi_z \in \text{Dom}(B)$, contradicting the fact that B is symmetric.

Hence $Y(w, z)$ is injective whenever $w, z \in \mathbb{C}_+$ or in \mathbb{C}_- . But then $Y^*(w, z) = Y(z, w)$ is also injective, proving that $Y(w, z)$ also always has dense range. This proves that $Y(z, w)$ is always a quasi-affinity of $\mathcal{B}(\ell^2(\mathbb{N}))$ whenever z, w are both in \mathbb{C}_+ or are both in \mathbb{C}_- . \square

Proof. (of Proposition 5.5)

If $z, w \in \Pi_\Gamma^+$ this follows from the observation that given any orthonormal basis $\{j_k\}$ of \mathcal{J} , and $z \in \Pi_\Gamma^+$, $\delta_k(\bar{z}) := \Gamma(z)j_k$ forms a basis for $\text{Ker}(B^* - \bar{z})$, and that

$$\Gamma(z) = \sum \langle \cdot, j_i \rangle \delta_i(\bar{z}),$$

so that

$$\Gamma^*(z)\Gamma(w) = [\langle \delta_j(\bar{z}), \delta_k(\bar{w}) \rangle]_{1 \leq j, k \leq n}.$$

The proof of the other half of the proposition is analogous. \square

For the remainder of this section we will assume that $n < \infty$, although many of our arguments generalize to the case $n = \infty$ without too much difficulty.

Lemma 5.10. *The sets $\Sigma_\Gamma^\pm = \mathbb{C}_\pm \setminus \Pi_\Gamma^\pm$ are contained in the zero-sets of non-zero analytic functions in \mathbb{C}_\pm (and hence are purely discrete with accumulation points lying only on $\mathbb{R} \cup \{\infty\}$).*

Proof. Choose any $w \in \Pi_\Gamma^+$. Let $\{j_k\}$ be an orthonormal basis of \mathcal{J} such that $\{j_k\}_{k=1}^{m_+}$ is an orthonormal basis of $\text{Ker}(\Gamma(w))^\perp$. Let $\{v_k\}_{k=1}^{m_+}$ be the basis of $\text{Ran}(\Gamma(w))$ defined by $v_k = \Gamma(w)j_k$ and set

$$D_w(z) := [\langle \Gamma(w)j_k, \Gamma(z)j_l \rangle]_{1 \leq k, l \leq m_+},$$

and let $\delta_w(z) := \det D_w(z)$. Then δ_w is analytic (as a function of z) in \mathbb{C}_+ and δ_w is not identically zero since $\delta_w(w) = \det D_w(w)$, and it is clear that by construction $D_w(w)$ is invertible. Now if $z \in \mathbb{C}_+$ is any point such that $\delta_w(z) \neq 0$ then $D_w(z)$ is invertible and hence $\Gamma(z)|_{\text{Ker}(\Gamma(w))^\perp}$ is invertible as a map onto its range. Let $\tilde{j}_k := P_z j_k$ where P_z projects onto $\text{Ker}(\Gamma(z))^\perp$. The \tilde{j}_k form a linearly independent set since otherwise the set of all

$$\Gamma(z)j_k = \Gamma(z)\tilde{j}_k,$$

would not be linearly independent, contradicting the fact that $\Gamma(z)|_{\text{Ker}(\Gamma(w))^\perp}$ is invertible. It follows that

$$\dim(\text{Ker}(\Gamma(z))^\perp) \geq m_+ = \max_{z \in \mathbb{C}_+} \dim(\text{Ker}(\Gamma(z))^\perp),$$

for any $z \in \mathbb{C}_+$ such that $\delta_w(z) \neq 0$, proving the claim. \square

Corollary 5.11. *Given any $w \in \Pi_\Gamma^\pm$ we have that the set*

$$\mathbb{C}_\pm \setminus \{z \in \mathbb{C}_\pm \mid \Gamma(z)^* \Gamma(w)|_{\text{Ker}(\Gamma(w))^\perp} \text{ is invertible} \},$$

is contained in the zero set of an analytic function which is not identically zero.

Lemma 5.12. *Suppose that $n < \infty$. If $m_+ = n$ then $\bigvee_{z \in \mathbb{C}_+} \Gamma(z)\mathcal{J} = \bigvee_{z \in \mathbb{C}_+} \text{Ker}(B^* - \bar{z})$. Similarly if $m_- = n$ then $\bigvee_{z \in \mathbb{C}_-} \Gamma(z)\mathcal{J} = \bigvee_{z \in \mathbb{C}_-} \text{Ker}(B^* - \bar{z})$. Consequently if $m_+ = n = m_-$ then the simplicity of B implies that $\bigvee_{z \in \mathbb{C} \setminus \mathbb{R}} \Gamma(z)\mathcal{J} = \mathcal{H}$.*

Proof. This is intuitively clear. Since B is simple, $\bigvee_{z \in \mathbb{C} \setminus \mathbb{R}} \text{Ker}(B^* - z)$ is dense in \mathcal{H} . By definition if $z \notin \Sigma_\Gamma^+$ and $m_+ = n$ then $\text{Ker}(B^* - \bar{z}) = \Gamma(z)\mathcal{J}$. By Lemma 5.10 the set Π_Γ^+ of all $z \in \mathbb{C}_+$ for which $\Gamma(z)$ is invertible is dense in \mathbb{C}_+ .

If $f \in \mathcal{H}$ and $f \perp \bigvee_{z \in \mathbb{C}_+} \Gamma(z)\mathcal{J}$ then $f \perp \text{Ker}(B^* - \bar{z})$ for all $z \in \Pi_\Gamma^+$. Let $\tilde{\Gamma}$ be a canonical model for B , and let $\tilde{f}(z) := \tilde{\Gamma}(z)^* f$. Since $f \perp \text{Ker}(B^* - \bar{z})$ for all $z \in \Pi_\Gamma^+$, the \mathcal{J} -valued analytic function $\tilde{f}(z)$ vanishes everywhere on Π_Γ^+ . Since this set is dense in \mathbb{C}_+ , $\tilde{f} = 0$ identically on \mathbb{C}_+ . This shows that $f \perp \bigvee_{z \in \mathbb{C}_+} \text{Ker}(B^* - \bar{z})$. The same argument in \mathbb{C}_- completes the proof. \square

Definition 5.13. We say that a quasi-model Γ is a *generalized* or *non-canonical model* for B if

$$\bigvee_{z \in \mathbb{C} \setminus \mathbb{R}} \text{Ran}(\Gamma(z)) = \mathcal{H}.$$

By Lemma 5.12, any full rank quasi-model (a rank (n, n) quasi-model) is a generalized model for B . The next proposition verifies that the linear maps Γ_A^w defined for $A \in \text{Ext}(B)$ and $w \in \mathbb{C} \setminus \mathbb{R}$ in equation (5.3) satisfy our definition of a quasi-model.

Proposition 5.14. *If $B \in \mathcal{S}_n(\mathcal{H})$ with Θ_B inner and $A \in \text{Ext}(B)$, then for any $w \in \mathbb{C} \setminus \mathbb{R}$ one can construct a generalized model Γ_A^w for B by defining $\mathcal{J} := \mathbb{C}^n$, $J_w : \mathcal{J} \rightarrow \text{Ker}(B^* - w)$ a bounded isomorphism and letting*

$$\Gamma_A^w(z) := P_{\mathcal{H}} U_{w, \bar{z}} J_w.$$

The quasi-model Γ_A^w has rank (n, m_+) if $w \in \mathbb{C}_+$ and rank (m_-, n) if $w \in \mathbb{C}_-$ where $0 \leq m_{\pm} \leq n$.

We will usually assume that J_w is chosen to be an isometry. Recall that if A is such that $A = b^{-1}(U)$ and $1 \notin \sigma_p(U)$, then $U_{wz} = P_{\mathcal{H}}(A - w)(A - \bar{z})^{-1}$, as in equation (5.1). In the exceptional case where $1 \in \sigma_p(U)$, U_{wz} is given by equation (5.2).

Proof. First, clearly Γ_A^w is anti-analytic on $\mathbb{C} \setminus \mathbb{R}$. Also as discussed previously, $\Gamma_A^w(\bar{z}) \in \text{Ker}(B^* - z)$ since $U_{w,z}$ maps $\text{Ker}(B^* - w)$ into $(\mathcal{K} \ominus \mathcal{H}) \oplus \text{Ker}(B_A^* - z)$ (as discussed at the beginning of this section). \square

Note that by construction $\Gamma_A^w(\bar{w}) = J_w$, which is invertible by assumption.

Given any $A \in \text{Ext}(B)$, we are free to choose $w \in \mathbb{C} \setminus \mathbb{R}$ in the construction of a quasi-model Γ_A^w associated with A . For the remainder of this paper we will choose $w = -i$ unless otherwise specified and define

$$\Gamma_A(z) := \Gamma_A^{-i}(z),$$

which (excluding the exceptional case) is equal to

$$P_{\mathcal{H}}(A + i)(A - \bar{z})^{-1}J_{-i},$$

and $\Gamma_A(i) = J_{-i}$. We will also simply write J for J_{-i} where $J = P_{-i}J : \mathbb{C}^n \rightarrow \text{Ker}(B^* + i)$, and usually we assume J is an isometry.

Remark 5.15. Suppose that the characteristic function Θ of B is inner. If this is the case then we will show that for any $A \in \text{Ext}(B)$, that $\bigvee_{z \in \mathbb{C}_-} \text{Ran}(\Gamma_A^w(\bar{z})) = \mathcal{H}$ for any $w \in \mathbb{C}_+$ and $\bigvee_{z \in \mathbb{C}_+} \text{Ran}(\Gamma_A^w(\bar{z})) = \mathcal{H}$ whenever $w \in \mathbb{C}_-$.

To see this note that in this case that B is unitarily equivalent to Z_{Θ} , which acts as multiplication by z in some model space K_{Θ}^2 . Suppose that $U : \mathcal{H} \rightarrow K_{\Theta}^2$ is this unitary transformation such that $U^*Z_{\Theta}U = B$. Let $C_{\Theta} = \dagger \circ \Theta^*$ be the canonical anti-linear isometry from K_{Θ}^2 onto $K_{\Theta^T}^2$, where T denotes transpose, as defined in [15, Claim 3]. The existence of C_{Θ} also follows from our Corollary 4.9.

Suppose that $w \in \mathbb{C}_+$. Then by Lemma 5.12, since $m_- = n$ for any Γ_A^w (because $\Gamma_A^w(\bar{w})$ is invertible),

$$\begin{aligned} \bigvee_{z \in \mathbb{C}_-} \text{Ran}(\Gamma_A^w(z)) &= \bigvee_{z \in \mathbb{C}_+} \text{Ker}(B^* - z) \\ &= U^* \bigvee_{z \in \mathbb{C}_+} \text{Ker}(Z_{\Theta}^* - z) \\ &= U^* \bigvee \{C_{\Theta}k_z^{\Theta^T}\} \\ &= U^*K_{\Theta}^2 = \mathcal{H}. \end{aligned}$$

Similarly if $w \in \mathbb{C}_-$ then

$$\begin{aligned} \bigvee_{z \in \mathbb{C}_+} \text{Ran}(\Gamma_A^w(z)) &= U^* \bigvee_{z \in \mathbb{C}_-} \text{Ker}(Z_{\Theta}^* - z) \\ &= U^* \bigvee \{k_z^{\Theta}\} \\ &= U^*K_{\Theta}^2 = \mathcal{H}. \end{aligned}$$

This proves that if Θ_B is inner, then every quasi-model Γ_A^w for $A \in \text{Ext}(B)$ and $w \in \mathbb{C} \setminus \mathbb{R}$ is a generalized model.

Example 5.16. (An example of Z_A with indices (n, n) where $m_+ = m < n$.)

Suppose that $B \in \mathcal{S}_n(\mathcal{H})$ and Θ_B is inner so that for any $A \in \text{Ext}(B)$ and $w \in \mathbb{C} \setminus \mathbb{R}$, Γ_A^w is a generalized model for B (see Remark 5.15 above).

Let $V :=$ the partial isometric extension of $b(B)$ to \mathcal{H} . Given any $C \in \overline{B_1(\mathbb{C}^{n \times n})}$ define

$$\hat{C} := \sum_{jk} C_{jk} \langle \cdot, u_j \rangle v_k,$$

where $\{u_j\}$ is an orthonormal basis of $\text{Ker}(V) = \text{Ker}(B^* - i)$ and $\{v_k\}$ an orthonormal basis of $\text{Ran}(V)^\perp = \text{Ker}(B^* + i)$. Let

$$V(C) := V + \hat{C},$$

a contractive extension of V and let (U_C, \mathcal{K}) be the minimal unitary dilation of $V(C)$. Choose $C = \mathbb{1}_m$ where $0 \leq m < n$ so that $\hat{C}u_j = 0$ for any $n \geq j > m$. Let us assume that $V(C)$ does not have 1 as an eigenvalue. This is the case, for example, if B is densely defined (see *e.g.* [2, Lemma 6.1.3]). Then it follows from [7, Proposition 6.1, Chapter 2], that 1 is not an eigenvalue of U so that $b^{-1}(U_C) =: A_C \in \text{Ext}(B)$ and $U_C = b(A_C)$. Define

$$\Gamma_C(z) := \Gamma_{A_C}^i(z) = P_{\mathcal{H}}(A_C - i)(A_C - \bar{z})^{-1}J_i,$$

where $J_i : \mathbb{C}^n \rightarrow \text{Ker}(B^* - i)$ is chosen to be an isometry such that $J_i e_k = u_k$, where $\{e_k\}$ is the standard orthonormal basis of \mathbb{C}^n . Now

$$\Gamma_C(i) = P_{\mathcal{H}}(A_C - i)(A_C + i)^{-1}J_i = P_{\mathcal{H}}b(A_C)P_{\mathcal{H}}J_i = V(C)J_i = \hat{C},$$

since $b(A_C) = U_C$ is an extension of $V(C)$. It follows that

$$\Gamma_C(i)e_j = 0,$$

for any $n \geq j > m$. Now given any $z \in \mathbb{C}_+$,

$$\begin{aligned} \Gamma_C(z) &= P_{\mathcal{H}}(A_C - i)(A_C - \bar{z})^{-1}J_i \\ &= P_{\mathcal{H}}(A_C + i)(A_C - \bar{z})^{-1}(A_C - i)(A_C - \bar{i})^{-1}P_{\mathcal{H}}J_i. \end{aligned} \quad (5.11)$$

Since both $z, i \in \mathbb{C}_+$, by dilation theory this is just equal to

$$\Gamma_C(z) = P_{\mathcal{H}}(A_C + i)(A_C - \bar{z})^{-1}P_{\mathcal{H}}b(A_C)P_{\mathcal{H}}J_i,$$

so that $\Gamma_C(z)e_j = 0$ for any $n \geq j > m$ as before. To see this note that since $U_C = b(A_C)$ is a dilation of $V(C)$, that for any $n \in \mathbb{N} \cup \{0\}$,

$$P_{\mathcal{H}}b(A_C)^n P_{\mathcal{H}} = (P_{\mathcal{H}}b(A_C)P_{\mathcal{H}})^n$$

It follows that

$$P_{\mathcal{H}}(A_C + i)^{-n}P_{\mathcal{H}} = (P_{\mathcal{H}}(A_C + i)^{-1}P_{\mathcal{H}})^n.$$

Given any $z \in \mathbb{C}_-$ that lies in the open ball of radius 1 about $z = -i$ we have that $(A_C - z)^{-1}$ can be expressed as a power series in $(A_C + i)^{-1}$, and it follows from this that the resolvent formula:

$$\begin{aligned} (z - w)P_{\mathcal{H}}(A_C - z)^{-1}(A_C - w)^{-1}P_{\mathcal{H}} &= P_{\mathcal{H}}(A_C - w)^{-1}P_{\mathcal{H}} - P_{\mathcal{H}}(A - z)^{-1}P_{\mathcal{H}} \\ &= (z - w)P_{\mathcal{H}}(A - z)^{-1}P_{\mathcal{H}}(A - w)^{-1}P_{\mathcal{H}}, \end{aligned}$$

holds for all $z, w \in \mathbb{C}_-$.

Hence $\Gamma(z)u_j$ is identically zero in \mathbb{C}_+ for any $n \geq j > n$ so that

$$m_+ = \max_{z \in \mathbb{C}_+} \text{Ker}(\Gamma(z))^\perp = m.$$

Similarly using $\Gamma = \Gamma_{AC}^{-i}$ instead, one can construct an example of Z_A with indices (n, n) where $n > m_-$.

6. CONSTRUCTION OF THE MODEL REPRODUCING KERNEL HILBERT SPACE

Given any quasi-model Γ for $B \in \mathcal{S}_n(\mathcal{H})$, we can construct a reproducing kernel Hilbert space \mathcal{H}_Γ as follows:

Definition 6.1. For $f \in \mathcal{H}$ define

$$\hat{f}(z) := \Gamma^*(z)f,$$

an analytic function on $\mathbb{C} \setminus \mathbb{R}$, and let $\mathcal{H}_\Gamma :=$ the vector space of all the functions \hat{f} .

Let $\mathcal{H}_\Gamma^{-1} = \bigvee_{z \in \mathbb{C} \setminus \mathbb{R}} \text{Ran}(\Gamma(z))$, $\mathcal{H}_\Gamma^{-1} \subset \mathcal{H}$. Then clearly \mathcal{H}_Γ is the set of all functions \hat{f} for $f \in \mathcal{H}_\Gamma^{-1}$, and if $f \perp \mathcal{H}_\Gamma^{-1}$ then $\hat{f} = 0$. We define an inner product on \mathcal{H}_Γ by

$$\langle \hat{f}, \hat{g} \rangle_\Gamma := \langle f, g \rangle,$$

whenever $f, g \in \mathcal{H}_\Gamma^{-1}$.

According to Definition 5.13, we call Γ a generalized model if $\mathcal{H}_\Gamma^{-1} = \mathcal{H}$.

We say that the reproducing kernel Hilbert space \mathcal{H}_Γ has the division property in \mathbb{C}_\pm if whenever $\hat{f} \in \mathcal{H}_\Gamma$ and $\hat{f}(w) = 0$ for $w \in \Pi_\Gamma^\pm$ we have that

$$\frac{\hat{f}(z)}{z - w} \in \mathcal{H}_\Gamma.$$

Proposition 6.2. *With the above inner product \mathcal{H}_Γ is a reproducing kernel Hilbert space of analytic functions on $\mathbb{C} \setminus \mathbb{R}$ with reproducing kernel*

$$k_w^\Gamma(z) = \Gamma(z)^* \Gamma(w),$$

and point evaluation vectors

$$k_w^\Gamma j = U_\Gamma \Gamma(w)j,$$

for $j \in \mathcal{J}$. If the rank of Γ is (m_+, m_-) then \mathcal{H}_Γ has the division property in \mathbb{C}_\pm whenever $m_\pm = n$.

The map $U_\Gamma : \mathcal{H} \rightarrow \mathcal{H}_\Gamma$ defined by $U_\Gamma f = \hat{f}$ is a co-isometry with initial space \mathcal{H}_Γ^{-1} , and is unitary if and only if Γ is a generalized model for B . If Γ is a generalized model then $Z_\Gamma := U_\Gamma B U_\Gamma^{-1}$ acts as multiplication by z on the domain $U_\Gamma \text{Dom}(B)$, and if either m_+ or m_- is equal to n then

$$\text{Dom}(Z_\Gamma) = \{\hat{f} \mid z\hat{f}(z) \in \mathcal{H}_\Gamma\}.$$

Recall that if Θ_B is inner then given any $A \in \text{Ext}(B)$, and $w \in \mathbb{C} \setminus \mathbb{R}$, any quasi-model Γ_A^w is a generalized model with indices (m_+, n) or (n, m_-) .

Proof. This is all fairly straightforward to check. First of all one should verify that $\|\hat{f}\|_\Gamma = 0$ implies that $f \perp \mathcal{H}_\Gamma^{-1}$, i.e. that $\hat{f}(z) = \Gamma(z)^* f = 0$ for all $z \in \mathbb{C} \setminus \mathbb{R}$. Indeed $\Gamma(z)^* f = 0$ for $z \in \mathbb{C} \setminus \mathbb{R}$ if and

only if $\langle f, \Gamma(z)j \rangle = 0$ for all $z \in \mathbb{C} \setminus \mathbb{R}$, and $j \in \mathcal{J}$ which happens if and only if $f \perp \text{Ran}(\Gamma(z))$ for all $z \in \mathbb{C} \setminus \mathbb{R}$, in other words $f \perp \mathcal{H}_\Gamma^{-1}$.

Now given any $j \in \mathcal{J}$ and $f \in \mathcal{H}_\Gamma^{-1}$,

$$\langle \hat{f}(w), j \rangle_{\mathcal{J}} = \langle f, \Gamma(w)j \rangle_{\mathcal{H}} = \langle \hat{f}, U_\Gamma \Gamma(w)j \rangle_\Gamma, \quad (6.1)$$

and it follows from this that for any $j \in \mathcal{J}$, $k_w j := U_\Gamma \Gamma(w)j$ are reproducing kernel vectors in \mathcal{H}_Γ and the reproducing kernel is given by

$$\begin{aligned} \langle k_w(z)j_1, j_2 \rangle_{\mathcal{J}} &= \langle k_w j_1, k_z j_2 \rangle_\Gamma = \langle \Gamma(w)j_1, \Gamma(z)j_2 \rangle_{\mathcal{H}} \\ &= \langle \Gamma(z)^* \Gamma(w)j_1, j_2 \rangle_{\mathcal{J}}. \end{aligned}$$

Now suppose U_Γ is unitary and define $Z_\Gamma := U_\Gamma B U_\Gamma^{-1}$ on $U_\Gamma \text{Dom}(B)$. Let us first show that Z_Γ acts as multiplication by z on its domain. If $f \in \text{Dom}(B)$ then

$$Z_\Gamma \hat{f} = U_\Gamma B f$$

so that for any $j \in \mathcal{J}$,

$$\langle (U_\Gamma B f)(z), j \rangle_{\mathcal{J}} = \langle B f, \Gamma(z)j \rangle_{\mathcal{H}} = \langle f, B^* \Gamma(z)j \rangle \quad (6.2)$$

$$= z \langle f, \Gamma(z)j \rangle = \langle z \hat{f}(z), j \rangle_{\mathcal{J}}, \quad (6.3)$$

showing that $Z_\Gamma \hat{f}(z) = z \hat{f}(z)$.

Now suppose that $m_+ = n$, and let's prove that \mathcal{H}_Γ has the division property in \mathbb{C}_+ . In this case if $\hat{f} \in \mathcal{H}_\Gamma$ and $\hat{f}(w) = 0$ then

$$0 = \langle \hat{f}(w), j \rangle = \langle f, \Gamma(w)j \rangle,$$

for any $j \in \mathcal{J}$. If $w \in \Pi_\Gamma^+$, then $\Gamma(w) : \mathcal{J} \rightarrow \text{Ker}(B^* - \overline{w})$ is onto which implies that $f \in \text{Ran}(B - w)$. Then $f = (B - w)g$, and $\hat{f} = (Z_\Gamma - w)\hat{g}$, or

$$\hat{g}(z) = \frac{\hat{f}(z)}{z - w}.$$

It remains to prove that if (without loss of generality) $m_+ = n$ and $\hat{f} \in \mathcal{H}_\Gamma$ is such that $z \hat{f}(z) \in \mathcal{H}_\Gamma$ then $\hat{f} \in \text{Dom}(Z_\Gamma)$. If \hat{f} and $z \hat{f} \in \mathcal{H}_\Gamma$ then so is $(z - w)\hat{f} =: \hat{g}$ for any fixed $w \in \Pi_\Gamma^+$, and some $g \in \mathcal{H}$. Since \hat{g} vanishes at w , it follows that $\Gamma^*(w)g = 0$, so that $g \perp \text{Ran}(\Gamma(w)) = \text{Ker}(B^* - \overline{w})$ since $w \in \Pi_\Gamma$. It follows that $g = (B - w)h$ for some $h \in \mathcal{H}$ so that $\hat{g}(z) = (z - w)\hat{h}(z)$ for any $z \in \mathbb{C} \setminus \mathbb{R}$. But since $\hat{g}(z) = (z - w)\hat{f}(z)$ it follows that $\hat{f} = \hat{h}$ so that $f = h \in \text{Dom}(B)$. \square

6.3. Alternate formulas for the Livsic characteristic function. In this subsection we pause to compute an alternate formula for the Livsic characteristic function. This will be useful, in particular, for computing formulas for the reproducing kernel of \mathcal{H}_Γ in the next subsection.

Suppose that $B \in \mathcal{S}_n(\mathcal{H})$ where $n < \infty$. As mentioned in the introduction the Livsic characteristic function of B is usually defined using

$$\begin{aligned} \{u_k\}_{k=1}^n &\quad \text{orthonormal basis of } \text{Ker}(B^* - i) \\ \{v_k\}_{k=1}^n &\quad \text{orthonormal basis of } \text{Ker}(B^* + i) \\ \{w_k(z)\}_{k=1}^n &\quad \text{arbitrary basis of } \text{Ker}(B^* - z) \end{aligned}$$

and

$$A(z) := [\langle w_j(z), v_k \rangle] \quad B(z) := [\langle w_j(z), u_k \rangle],$$

by

$$\Theta_B(z) = b(z)B(z)^{-1}A(z).$$

Here is an alternate formula that is sometimes useful. Let A be a canonical self-adjoint extension of B and let

$$w_j(z) := \Gamma_A^i(\bar{z})e_j \in \text{Ker}(B^* - z),$$

and choose $v_j := \Gamma_A^i(i)e_j = (A - i)(A + i)^{-1}u_j$, where recall we choose $J_i : \mathbb{C}^n \rightarrow \text{Ker}(B^* - i)$ so that $J_i e_j = u_j$, $\{e_j\}$ is the standard orthonormal basis of \mathbb{C}^n , and J_i is an isometry.

Then it follows that

$$\begin{aligned} \langle w_j(z), v_k \rangle &= \langle (A - i)(A - z)^{-1}u_j, (A - i)(A + i)^{-1}u_k \rangle \\ &= \langle u_j, (A - i)(A - \bar{z})^{-1}u_k \rangle = \langle u_j, w_k(\bar{z}) \rangle. \end{aligned} \quad (6.4)$$

This shows that

$$A(z) = [\langle u_j, w_k(\bar{z}) \rangle],$$

and a similar calculation shows that

$$B(z) = [\langle v_j, w_k(\bar{z}) \rangle].$$

It follows that $A(\bar{z})^* = B(z)$.

6.4. Reproducing Kernel formulas for \mathcal{H}_Γ . Let Γ be a generalized model for B of rank (m_+, m_-) where at least one of m_\pm is equal to n . Then by Proposition 6.2 we have an isometry $U_\Gamma : \mathcal{H} \rightarrow \mathcal{H}_\Gamma$ such that

$$U_\Gamma B = Z_\Gamma U_\Gamma,$$

so that Z_Γ is unitarily equivalent to B .

For any $w \in \mathbb{C} \setminus \mathbb{R}$ let P_w be the projection onto $\text{Ran}(B - w) = \text{Ker}(B^* - \bar{w})^\perp$, and let $Q_w := U_\Gamma P_w U_\Gamma^*$, the projection onto $\text{Ran}(Z_\Gamma - w)$. Now define

$$L_w := U_\Gamma b_{\bar{w}}(B)P_w U_\Gamma^* = b_{\bar{w}}(Z_\Gamma)Q_w,$$

the partial isometric extension of $b_{\bar{w}}(Z_\Gamma)$ to all of \mathcal{H}_Γ . It is clear that

$$L_w = Q_{\bar{w}} b_{\bar{w}}(Z_\Gamma) Q_w,$$

and that $L_w^* = L_{\bar{w}}$.

We can now calculate formulas for the reproducing kernel of \mathcal{H}_Γ , using the same procedure as in [4, Section 4]. Let $k_w(z) = k_w^\Gamma(z)$ denote the reproducing kernel of \mathcal{H}_Γ . Now given any $u, v \in \mathcal{J}$ and $\alpha \in \mathbb{C} \setminus \mathbb{R}$,

$$\begin{aligned} \langle (L_\alpha^* k_w)(z)u, v \rangle &= \langle L_\alpha^* k_w u, k_z v \rangle \\ &= \langle k_w u, L_\alpha k_z v \rangle = \overline{\langle b_{\bar{\alpha}}(Z_\Gamma) Q_\alpha k_z v, k_w u \rangle} \\ &= \overline{b_{\bar{\alpha}}(w)} \langle k_w u, Q_\alpha k_z v \rangle \\ &= \frac{1}{b_\alpha(w)} (\langle k_w(z)u, v \rangle - \langle ((1 - Q_\alpha)k_w)(z)u, v \rangle). \end{aligned} \quad (6.5)$$

But also,

$$\begin{aligned} \langle (L_\alpha^* k_w)(z)u, v \rangle &= \langle (L_{\bar{\alpha}} k_w)(z)u, v \rangle = b_\alpha(z) \langle Q_{\bar{\alpha}} k_w u, k_z v \rangle \\ &= b_\alpha(z) (\langle k_w(z)u, v \rangle - \langle ((1 - Q_{\bar{\alpha}})k_w)(z)u, v \rangle). \end{aligned} \quad (6.6)$$

Solving for $\langle k_w(z)u, v \rangle$ and using that $u, v \in \mathcal{J}$ were arbitrary yields:

$$k_w^\Gamma(z) = \frac{((1 - Q_\alpha)k_w)(z) - b_\alpha(z)\overline{b_\alpha(w)}((1 - Q_{\bar{\alpha}})k_w)(z)}{1 - b_\alpha(z)\overline{b_\alpha(w)}}, \quad (6.7)$$

for any $\alpha \in \mathbb{C} \setminus \mathbb{R}$.

Now suppose Γ is a rank (m_-, n) quasi-model for B and that Z_Γ is unitarily equivalent to B . This happens for example if $\Gamma = \Gamma_A$ for some $A \in \text{Ext}(B)$. Also choose $\mathcal{J} := \mathbb{C}^n$, and $J : \mathbb{C}^n \rightarrow \text{Ker}(B^* + i)$ to be an isometry, and $\alpha = i$ in equation (6.7).

Let $\{u_k\}$ be an orthonormal basis for $\text{Ker}(B^* - i)$ such that $\{u_k\}_{k=1}^{n_+}$ is a basis for $\text{Ran}(\Gamma(-i))$, and let $\{v_k\}_{k=1}^n$ be an orthonormal basis for $\text{Ker}(B^* + i)$ such that $v_k = Je_k$, and $\{e_k\}$ is an orthonormal basis of \mathbb{C}^n . We assume here that J is an isometry.

Using that $1 - Q_{-i} = \sum_{l=1}^n \langle \cdot, \hat{u}_l \rangle \hat{u}_l$ we can compute:

$$\begin{aligned} \langle ((1 - Q_{-i})k_w)(z)e_j, e_k \rangle &= \sum_{l=1}^{n_+} \langle k_w e_j, \hat{u}_l \rangle \langle \hat{u}_l, k_z e_k \rangle_\Gamma \\ &= \sum_{l=1}^{n_+} \langle U_\Gamma \Gamma(w)e_j, U_\Gamma u_l \rangle \langle U_\Gamma u_l, U_\Gamma \Gamma(z)e_k \rangle \\ &= \sum_{l=1}^{n_+} \langle \Gamma(w)e_j, u_l \rangle \langle u_l, \Gamma(z)e_k \rangle. \end{aligned}$$

Let $w_j(\bar{w}) := \Gamma(w)e_j \in \text{Ker}(B^* - \bar{w})$, and define the $n \times n$ matrix

$$\alpha(z) := [\langle u_j, w_k(\bar{z}) \rangle]. \quad (6.8)$$

Hence the above can be written:

$$\langle ((1 - Q_{-i})k_w)(z)e_j, e_k \rangle = \sum_{l=1}^n \langle w_j(\bar{w}), u_l \rangle \langle u_l, w_k(\bar{z}) \rangle.$$

Compare this to

$$\begin{aligned} (\alpha(z)\alpha(w)^* e_j, e_k) &= \sum_{l=1}^n (e_j, \alpha(w)e_l) (\alpha(z)e_l, e_k) \\ &= \sum_{l=1}^n \langle w_j(\bar{w}), u_l \rangle \langle u_l, w_k(\bar{z}) \rangle. \end{aligned}$$

This proves that

$$((1 - Q_{-i})k_w(z)) = \alpha(z)\alpha(w)^*. \quad (6.9)$$

A similar calculation shows that since $(1 - Q_i) = \sum_{l=1}^n \langle \cdot, \hat{v}_l \rangle \hat{v}_l$ we get that

$$\langle ((1 - Q_i)k_w)(z)e_j, e_k \rangle = \sum_{l=1}^n \langle w_j(\overline{w}), v_l \rangle v_l w_k(\overline{z}).$$

If we take $\beta(z) := [\langle v_l, w_k(\overline{z}) \rangle]$ then as before it is not hard to check that

$$(\beta(z)\beta(w)^*e_j, e_k) = \sum_{l=1}^n \langle w_j(\overline{w}), v_l \rangle \langle v_l, w_k(\overline{z}) \rangle,$$

which shows that

$$((1 - Q_i)k_w)(z) = \beta(z)\beta(w)^*. \quad (6.10)$$

It follows that our formula for the reproducing kernel in \mathcal{H}_Γ can be written:

$$k_w^\Gamma(z) = \frac{\beta(z)\beta(w)^* - b(z)\overline{b(w)}\alpha(z)\alpha(w)^*}{1 - b(z)\overline{b(w)}}. \quad (6.11)$$

Now in the case where both $z, w \in \Pi_\Gamma$ (in particular for Γ_A we have that Π_A^+ is dense in \mathbb{C}_+) we have that $\{w_j(\overline{z})\}$ and $\{w_j(\overline{w})\}$ are bases for $\text{Ker}(B^* - \overline{z})$ and $\text{Ker}(B^* - \overline{w})$ respectively, so that for such z, w we have $\beta = B$ and $\alpha = A$, where A, B are the matrices in the definition of Θ_B (see Subsection 6.3),

$$\Theta_B(z) = b(z)B(z)^{-1}A(z).$$

Hence for any $z, w \in \Pi_\Gamma$

$$k_w^\Gamma(z) = B(z) \left(\frac{\mathbb{1} - \Theta_B(z)\Theta_B(w)^*}{1 - b(z)\overline{b(w)}} \right) B(w)^*. \quad (6.12)$$

Also observe that by the formula (6.11) we have that

$$k_i^\Gamma(z) = B(z)B(i)^* = B(z),$$

since $B(i) = [\langle Je_l, \Gamma(i)e_k \rangle] = [\langle Je_l, Je_k \rangle] = \mathbb{1}$. Also we have that $k_i(z) = \Gamma^*(z)\Gamma(i) = \Gamma(z)^*J$ so that $B(z) = \Gamma(z)^*J$.

7. CYCLICITY

The goal of this section is to show that the characteristic function Θ_B of B is inner implies that $\text{Ker}(B^* - w)$ is cyclic for any $A \in \text{Ext}(B)$. This will enable us, in the subsequent section, to extend the isometry $U_A : \mathcal{H} \rightarrow \mathcal{H}_A$ to an isometry $V_A : \mathcal{K} \rightarrow \mathcal{K}_A$ where A is self-adjoint in \mathcal{K} , $\mathcal{K}_A \supset \mathcal{H}_A$ is a larger reproducing kernel Hilbert space on $\mathbb{C} \setminus \mathbb{R}$ containing \mathcal{H}_A , and $V_A|_{\mathcal{H}_A} = U_A$. This larger space \mathcal{K}_A contains information about the extension $A \in \text{Ext}(B)$ that will be key for our characterization of $\text{Ext}(B)$.

Here we say that a subspace $S \subset \mathcal{H}$ is cyclic for $A \in \text{Ext}(B)$ if

$$\bigvee vN(A)S = \mathcal{H},$$

where $vN(A)$ is the von Neumann algebra generated by the unitary operator $b(A)$.

It will be convenient to apply some of the dilation theory for contractions as developed in [7]. The tools we are going to use are described below:

Given a contraction $T \in B(\mathcal{H})$, recall that the defect indices of T are defined to be the pair of positive integers $(\mathfrak{d}_T, \mathfrak{d}_{T^*})$ where

$$\mathfrak{d}_T := \dim \left(\overline{\text{Ran}(1 - T^*T)} \right).$$

Namely $\mathfrak{d}_T := \dim(\mathfrak{D}_T)$ where

$$\mathfrak{D}_T := \text{Ran} \left(D_T = \sqrt{1 - T^*T} \right).$$

Given $B \in \mathcal{S}_1(\mathcal{H})$, we will be studying the contraction

$$V := b_w(B)Q_w$$

where Q_w is the projection onto $\text{Ran}(B - \overline{w}) = \text{Ker}(B^* - w)^\perp$ for some fixed $w \in \mathbb{C} \setminus \mathbb{R}$ and $b_w(B)$ is the w -Cayley transform of B ,

$$b_w(z) = \frac{z - w}{z - \overline{w}}.$$

This is a partial isometry, and it is clear that the defect indices of V are equal to the deficiency indices of $b_w(B)$, namely (n, n) . A contraction is called c.n.u. (completely non-unitary) if it has no non-trivial unitary restriction. It is clear that since B is simple, this implies that V is c.n.u. The model theory of Nagy-Foias [7] associates a contractive operator-valued function Θ_T called the Nagy-Foias characteristic function of T , to any c.n.u. contraction T . This function is defined by

$$\Theta_T(z) := (-T + zD_{T^*}(1 - zT^*)^{-1}D_T)|_{\mathfrak{D}_T}.$$

In our case where $T = V$ is a partial isometry, this expression simplifies to:

$$\Theta_V(z) = zP_-(1 - zV^*)^{-1}P_+,$$

where P_+, P_- are the projectors onto $\mathfrak{D}_V = \text{Ker}(B^* - w)$ and $\mathfrak{D}_{V^*} = \text{Ker}(B^* - \overline{w})$ respectively. Since V is a partial isometry, in the case where $w = i$, the Nagy-Foias characteristic function Θ_V of $V = b_i(B)Q_w$ coincides with the Livsic characteristic function,

$$\theta_{b_i(B)} := \Theta_B \circ b_i^{-1},$$

of the isometric linear transformation $b_i(B)$, as shown for example in [2, Section 6].

Now recall that any contraction T acting on \mathcal{H} has a minimal unitary dilation U acting on some larger Hilbert space $\mathcal{K} \supset \mathcal{H}$. Recall that a unitary U on $\mathcal{K} \supset \mathcal{H}$ is called a unitary dilation of T if for any $n \in \mathbb{N} \cup \{0\}$ we have that

$$T^n = P_{\mathcal{H}}U^n|_{\mathcal{H}}.$$

Such a dilation is called minimal if \mathcal{K} is the smallest reducing subspace for U containing \mathcal{H} , and the minimal unitary dilation of T is unique up to a unitary transformation that fixes the Hilbert space \mathcal{H} [16, Theorem 4.3]. Since our contraction $V = b_w(B)Q_w$ is c.n.u. (because B is simple), it follows from [7, II.6.4], that the spectral measure of the minimal unitary dilation U of V is equivalent to Lebesgue measure. This just means that any of the positive Borel measures defined by $\sigma(\Omega) = \langle \chi_\Omega(U)f, f \rangle$, where $\Omega \subset \mathbb{T}$ is a Borel set, are equivalent (have the same sets of measure zero) to Lebesgue measure. Here χ_Ω denotes the characteristic function of the Borel set Ω , and $\chi_\Omega(U)$ is a projection by the functional calculus for unitary operators. It follows that U has no eigenvalues so that $b_w^{-1}(U)$ is a densely defined non-canonical self-adjoint extension of B . Moreover the fact that U is minimal implies that $\mathcal{K} \ominus \mathcal{H}$ contains no non-trivial reducing subspace S for U

(since otherwise $U|_{\mathcal{K} \ominus S}$ would be the minimal unitary dilation of V). Hence

$$b_w^{-1}(U) \in \text{Ext}(B).$$

Now as in [7, II.2] set

$$\mathcal{L} := \overline{(U - V)\mathcal{H}} = \bigvee U \text{Ker}(B^* - w),$$

and let

$$\mathcal{R}_* := \mathcal{K} \ominus \left(\overline{\bigoplus_{n \in \mathbb{Z}} U^n \mathcal{L}} \right) = \mathcal{K} \ominus \left(\overline{\bigoplus_{n \in \mathbb{Z}} U^n \text{Ker}(B^* - w)} \right).$$

Now by [7, Proposition 2.1 VI.2], the Nagy-Foias characteristic function Θ_V is a unitary if and only if both $V^n \rightarrow 0$ and $(V^*)^k \rightarrow 0$ in the strong operator topology. Note that if $n < \infty$ then since V has equal defect indices, the only way Θ_V can be an isometry is if it is in fact unitary, *i.e.* inner. Since Θ_V coincides with the Livsic characteristic function of $b_w(B)$ (this is a consequence of the fact that V is a partial isometry, as discussed above), we conclude that Θ_B is inner if and only if both $V^k \rightarrow 0$ strongly and $(V^*)^k \rightarrow 0$ strongly. In the notation of [7], if Θ_B is inner so that $V^k \rightarrow 0$ and $(V^*)^k \rightarrow 0$ strongly, and V has defect indices (n, n) , V is called a contraction of class $C_0(n)$.

By [7, II.3.1] the projection P_* onto \mathcal{R}_* can be calculated by the formula:

$$P_* h = \lim_{n \rightarrow \infty} U^{-n} V^n h. \quad (7.1)$$

Note that $\text{Ker}(B^* - w)$ is cyclic for $b_w^{-1}(U) \in \text{Ext}(B)$ if and only if $P_* = 0$.

Theorem 7.1. *Suppose $B \in \mathcal{S}_n(H)$, Q_w is the projection onto $\text{Ran}(B - \overline{w})$, and $P_w = 1 - Q_w$ projects onto $\text{Ker}(B^* - w)$. Let $V = b_w(B)Q_w$, U the minimal unitary dilation of V , and $A = b_w^{-1}(U) \in \text{Ext}(B)$. Then for any $h \in \mathcal{H}$,*

$$(1 - P_*)h = \sum_{j=0}^{\infty} U^{-j} P_w U^j h = \sum_{j=0}^{\infty} U^{-j} P_w V^j h. \quad (7.2)$$

Lemma 7.2. *Let $B \in \mathcal{S}_n(\mathcal{H})$, $A \in \text{Ext}(B)$. Given any $h \in \mathcal{H}$ then for any $k \in \mathbb{N}$:*

$$h = \sum_{j=0}^k b_w^\dagger(A)^j P_w (b_w(B)Q_w)^j h + b_w^\dagger(A)^{k+1} (b_w(B)Q_w)^{k+1} h. \quad (7.3)$$

In the above recall that $b_w(z) := \frac{z-w}{z-\overline{w}}$ and $b_w^\dagger(z) = \overline{b_w(\overline{z})} = \frac{z-\overline{w}}{z-w}$.

Proof. This clearly holds if $h \in \text{Ran}(B - \overline{w})^\perp$. If $h \perp \text{Ker}(B^* - w)$ then

$$h = Q_w h = b_w^\dagger(B) h_1,$$

for some $h_1 \in \text{Ran}(B - w) = \text{Dom}(b_w^\dagger(B))$. Now

$$h_1 = Q_w h_1 + P_w h_1,$$

and if we define $h_2 := Q_w h_1$ then $h_2 = b_w^\dagger(B) h_3$ for some $h_3 \in \text{Ran}(B - w)$. Now

$$h_3 = b_w(B) h_2 = b_w(B) Q_w h_1 = b_w(B) Q_w b_w(B) Q_w h = (b_w(B) Q_w)^2 h,$$

and

$$h = b_w^\dagger(B)h_1 = b_w^\dagger(B)(h_2 + P_w h_1) \quad (7.4)$$

$$= b_w^\dagger(B)(P_w h_1 + b_w^\dagger(B)h_3) \quad (7.5)$$

$$= b_w^\dagger(A)(P_w h_1 + b_w^\dagger(A)h_3) \quad (7.6)$$

$$= b_w^\dagger(A)P_w b_w(B)Q_w h + b_w^\dagger(A)^2(b_w(B)Q_w)^2 h. \quad (7.7)$$

Repeating this process k times yields $h_{2k+1} = (b_w(B)Q_w)^{k+1} h$ and one obtains the formula stated above, namely,

$$h = \sum_{j=0}^k b_w^\dagger(A)^j P_w (b_w(B)Q_w)^j h + b_w^\dagger(A)^{k+1} (b_w(B)Q_w)^{k+1} h.$$

□

Proof. (Theorem 7.1) In the case where $A = b_w^{-1}(U)$ where U is the minimal unitary dilation of $V = b_w(B)Q_w$, the formula (7.3) becomes:

$$\begin{aligned} h &= \sum_{j=0}^k U^{-j} P_w V^j h + U^{-(k+1)} V^{k+1} h \\ &= \sum_{j=0}^k U^{-j} P_w U^j h + U^{-(k+1)} V^{k+1} h \end{aligned} \quad (7.8)$$

Now we use the formula (7.1) of Nagy-Foias to conclude that if $A = b_w^{-1}(U)$ where U is the minimal unitary dilation of V , that $U^{-(k+1)} V^{k+1} h \rightarrow P_* h$, proving the formula (7.2) and the theorem. □

Corollary 7.3. *Suppose that $B \in \mathcal{S}_n(\mathcal{H})$. Then $\text{Ker}(B^* - w)$ and $\text{Ker}(B^* - \overline{w})$ are cyclic for every $A \in \text{Ext}(B)$ if and only if Θ_B is inner. If Θ_B is inner then the formulas*

$$h = \sum_{j=0}^{\infty} b_w^\dagger(A)^j P_w (b_w(B)Q_w)^j h, \quad (7.9)$$

hold for any $A \in \text{Ext}(B)$ and $h \in \mathcal{H}$.

Remark 7.4. Let $\{w_j\}$ be some fixed orthonormal basis of $\text{Ker}(B^* - w)$, and let $J_w : \mathbb{C}^n \rightarrow \text{Ker}(B^* - w)$ be defined by $J_w e_k = w_k$, where $\{e_k\}$ is an orthonormal basis of \mathbb{C}^n . Consider L_Σ^2 where Σ is the $\mathbb{C}^{n \times n}$ matrix-valued positive Borel measure defined by $\Sigma(\Omega) = J_w^* P_w P_A(\Omega) P_w J_w$, $P_A(\Omega) := \chi_\Omega(A)$, where χ_Ω is the characteristic function of the Borel set Ω . The above corollary shows in particular that for any fixed $h \in \mathcal{H}$ there is a vector function $\vec{f} = (f_1, \dots, f_n) \in L_\Sigma^2$ such that

$$h = f_1(A)w_1 + f_2(A)w_2 + \dots + f_n(A)w_n,$$

and that, remarkably, this equation holds independently of the choice of $A \in \text{Ext}(B)$, i.e. the same \vec{f} works for all $A \in \text{Ext}(B)$ when h is held fixed. Although we will not pursue this in this paper, this fact can be used to provide a new proof, and potentially a slight extension of the Alexandrov isometric measure theorem, [17, Theorem 2].

Proof. By Lemma 7.2, given any $A \in \text{Ext}(B)$ and $h \in \mathcal{H}$,

$$h = \sum_{j=0}^k b_w^\dagger(A)^j P_w (b_w(B)Q_w)^j h + b_w^\dagger(A)^{k+1} (b_w(B)Q_w)^{k+1} h.$$

Hence to prove the formula (7.9), it suffices to show that $\|(b_w(B)Q_w)^k h\| = \|b_w^\dagger(A)^k (b_w(B)Q_w)^k h\| \rightarrow 0$.

If Θ_B is inner then $V^n \rightarrow 0$ strongly (where recall $V = b_w(B)Q_w$) so that

$$0 = \lim_{n \rightarrow \infty} \|V^n h\|,$$

and so the formula (7.9) holds. If $A = b_w^{-1}(U)$, then the fact that $\text{Ker}(B^* - w)$ is cyclic follows from the fact that $\mathcal{R}_* = \{0\}$. For arbitrary $A \in \text{Ext}(B)$, the formula (7.9) shows that the cyclic subspace S_w for any fixed $A \in \text{Ext}(B)$ generated by $\text{Ker}(B^* - w)$ contains \mathcal{H} . Hence if A is self-adjoint in \mathcal{K} , then $S_w = \mathcal{K}$, as otherwise $\mathcal{K} \ominus S_w$ would be a non-trivial subspace of $\mathcal{K} \ominus \mathcal{H}$ which is reducing for A (this contradicts one of our assumptions on $\text{Ext}(B)$). This proves that $\text{Ker}(B^* - w)$ is cyclic for any $A \in \text{Ext}(B)$.

Conversely if $\text{Ker}(B^* - w)$ is cyclic for any $A \in \text{Ext}(B)$, then it is cyclic for $b_w^{-1}(U)$ where U is the minimal unitary dilation of $V = b_w(B)Q_w$, and it follows from the definition of R_* that $P_* = 0$, and hence $T^n \rightarrow 0$ strongly. If $n < \infty$ this implies T is a contraction of class $C_0(n)$, implying that the characteristic function Θ_B of B is inner as discussed previously. If $n = \infty$ our assumption that $\text{Ker}(B^* - \overline{w})$ is cyclic also implies that $(T^*)^k \rightarrow 0$ strongly as well so that we get that Θ_B is inner. \square

Note that the above proof also shows:

Corollary 7.5. *If $B \in \mathcal{S}_n(\mathcal{H})$, $n < \infty$, and there is a $w \in \mathbb{C} \setminus \mathbb{R}$ such that $\text{Ker}(B^* - w)$ is cyclic for every $A \in \text{Ext}(B)$, then Θ_B is inner.*

8. A LARGER REPRODUCING KERNEL HILBERT SPACE $\mathcal{K}_A \supset \mathcal{H}_A$

Definition 8.1. Given any $A \in \text{Ext}(B)$, let

$$\Omega_A(z) := U_{-i,z} J, \tag{8.1}$$

where recall that provided $A = b^{-1}(U)$ and U does not have 1 as an eigenvalue then

$$U_{-i,z} J = (A + i)(A - \overline{z})^{-1} J,$$

where recall that $J = J_{-i} = P_{-i} J_{-i}$ and $J : \mathbb{C}^n \rightarrow \text{Ker}(B^* + i)$. In the exceptional case where $A \in \text{Ext}(B)$ is defined using a unitary extension U of $b(B)$ and $1 \in \sigma_p(U)$, recall that $U_{w,z}$ is given by formula (5.2). We will assume in this section that J is an isometry. Note that

$$\Gamma_A(z) = P_{\mathcal{H}} \Omega_A(z). \tag{8.2}$$

We define a new reproducing kernel Hilbert space K_A as the abstract \mathbb{C}^n -valued reproducing kernel Hilbert space on $\mathbb{C} \setminus \mathbb{R}$ with reproducing kernel

$$K_w(z) := \Omega(z)^* \Omega(w)$$

The existence of \mathcal{K}_A follows from the fact that $K_w(z)$ is a positive kernel function, and the abstract theory of reproducing kernel Hilbert spaces [18, Theorem 10.11].

Observe that the difference

$$K_w(z) - k_w(z) = \Omega(z)^*(\mathbb{1} - P_{\mathcal{H}})\Omega(w),$$

is a positive kernel function. The theory of reproducing kernel Hilbert spaces then implies that \mathcal{H}_A is contractively contained in \mathcal{K}_A [18, Theorem 10.20].

For $\vec{v} \in \mathbb{C}^n$ the function $K_w\vec{v}$ defined by

$$K_w\vec{v}(z) := K_w(z)\vec{v},$$

is a point evaluation vector in \mathcal{K}_A , *i.e.*

$$\langle h, K_w\vec{v} \rangle_{\mathcal{K}_A} = (h(w), \vec{v})_{\mathbb{C}^n},$$

for any $h \in \mathcal{K}_A$.

Definition 8.2. Suppose that Θ_B is inner. Given $A \in \text{Ext}(B)$ self-adjoint in $\mathcal{K} \supset \mathcal{H}$, recall that we define $U_A : \mathcal{H} \rightarrow \mathcal{H}_A$ by

$$U_A(f)(z) = \hat{f}(z) = \Gamma(z)^*f.$$

Now define a linear map $V_A : \mathcal{K} \rightarrow \mathcal{K}_A$ by

$$(V_A f)(z) = \Omega_A(z)^*f,$$

for $f \in \mathcal{K}$.

Note that if $g \in \mathcal{H}$ that

$$(V_A g)(z) = J^*(A - z)^{-1}(A - i)g = \Gamma^*(z)g = (U_A g)(z),$$

so that for any $g \in \mathcal{H}$,

$$U_A g(z) = V_A g(z).$$

Hence if $E_A : \mathcal{H}_A \rightarrow \mathcal{K}_A$ is the contractive embedding then

$$V_A P_{\mathcal{H}} = E_A U_A. \tag{8.3}$$

Also observe that if $\vec{u} \in \mathbb{C}^n$, then

$$K_w\vec{u} = V_A \Omega(w)\vec{u},$$

is the \vec{u} point-evaluation vector in \mathcal{K}_A at w .

Proposition 8.3. *The linear map $V_A : \mathcal{K} \rightarrow \mathcal{K}_A$ is an isometry of \mathcal{K} onto \mathcal{K}_A . Hence if $h \in \mathcal{H}$, then*

$$\|V_A h\|_{\mathcal{K}_A} = \|h\| = \|U_A h\|_{\mathcal{H}_A},$$

so that $\mathcal{H}_A \subset \mathcal{K}_A$ isometrically and $U_A = V_A|_{\mathcal{H}}$.

Proof. Recall that since we assume that B is such that Θ_B is inner, Corollary 7.3 implies that $\text{Ker}(B^* + i)$ is cyclic for A .

Since $\text{Ker}(B^* + i)$ is cyclic, \mathcal{K} is spanned by vectors of the form $\Omega(w)J\vec{v}$ for $w \in \mathbb{C} \setminus \mathbb{R}$ and $\vec{v} \in \mathbb{C}^n$. In particular for any $\vec{v} \in \mathbb{C}^n$, the vector $V_A \Omega(w)\vec{v} \in \mathcal{K}_A$ since

$$(V_A \Omega(w)\vec{v})(z) := (\Omega(z)^* \Omega(w))\vec{v} = K_w(z)\vec{v},$$

and $K_w \vec{v} \in \mathcal{K}_A$. The set of all point evaluation vectors $K_w \vec{v}$, $K_w \vec{v}(z) := K_w(z) \vec{v}$ for $w \in \mathbb{C} \setminus \mathbb{R}$ are by definition dense in \mathcal{K}_A so that this also proves V_A is onto \mathcal{K}_A .

To see that V_A is an isometry use that vectors of the form $f = \sum_j c_j \Omega(w_j) \vec{v}_j$, for $\vec{v}_j \in \mathbb{C}^n$ and $w_j \in \mathbb{C}$ are dense in \mathcal{K} , so that

$$\langle f, f \rangle = \sum_{ij} c_i \bar{c}_j \langle \Omega(w_i) \vec{v}_i, \Omega(w_j) \vec{v}_j \rangle_{\mathcal{K}} \quad (8.4)$$

$$= \sum_{ij} c_i \bar{c}_j \langle K_{w_i}(w_j) \vec{v}_i, \vec{v}_j \rangle_{\mathbb{C}^n} \quad (8.5)$$

$$= \sum_{ij} c_i \bar{c}_j \langle K_{w_i} \vec{v}_i, K_{w_j} \vec{v}_j \rangle_{\mathcal{K}_A} \quad (8.6)$$

$$= \langle V_A f, V_A f \rangle_{\mathcal{K}_A}. \quad (8.7)$$

Now if $h \in \mathcal{H}$, then

$$\|E_A U_A h\|_{\mathcal{K}_A} = \|V_A h\|_{\mathcal{K}_A} = \|h\| = \|U_A h\|_{\mathcal{H}_A}.$$

Hence the contractive embedding $E_A : \mathcal{H}_A \rightarrow \mathcal{K}_A$ is actually an isometric inclusion, and $\mathcal{H}_A \subset \mathcal{K}_A$ as a Hilbert subspace. □

8.4. Cauchy transforms and characteristic functions for $A \in \text{Ext}(B)$. For any $A \in \text{Ext}(B)$, let $U := b(A)$ be the corresponding unitary extension of $V := b(B)$, and define σ_U as the $\mathbb{C}^{n \times n}$ matrix-valued measure on the unit circle \mathbb{T} given by

$$\sigma_U(\Omega) = \pi J^* P_U(\Omega) J,$$

where $P_U(\Omega) := \chi_{\Omega}(U)$ is the projection-valued measure of U defined using the functional calculus and recall that $J : \mathbb{C}^n \rightarrow \text{Ker}(B^* + i) = \text{Ker}(V)$ is a fixed isometry. We also define the $\mathbb{C}^{n \times n}$ positive matrix-valued measure on \mathbb{R} , Σ_A by

$$\Sigma_A(\Omega) := \int_{\Omega} \pi(1 + t^2) J^* P_A(dt) J,$$

and note that if $\sigma_A(\Omega) := J^* P_A(\Omega) J$, then $\sigma_A = \sigma_U \circ b$, where $b(z) = \frac{z-i}{z+i}$ as before.

Definition 8.5. If $A \in \text{Ext}(B)$ with $A = b^{-1}(U)$, let $\Phi[A; B]$ be the contractive analytic function on \mathbb{C}_+ corresponding to the pair $(\sigma_U(\{1\}), \Sigma_A)$ as described in Section 4. When there is no chance of confusion we will suppress dependence on B and use the simplified notation Φ_A for $\Phi[A; B]$. We call $\Phi[A; B]$ the characteristic function of A relative to B , or simply the characteristic function of A when it is clear which B is used in the definition of $\Phi[A; B]$.

In more detail, if $\phi := \phi[U; V]$, then

$$\text{Re}(g_{\phi}(z)) = \int_{\mathbb{T}} \text{Re} \left(\frac{\alpha + z}{\alpha - z} \right) \sigma_U(d\alpha),$$

where

$$\phi = \frac{g_{\phi} - \mathbb{1}}{g_{\phi} + \mathbb{1}}$$

Equivalently if we impose the normalization condition discussed in Section 4,

$$g_\phi(z) = \int_{\mathbb{T}} \frac{\alpha + z}{\alpha - z} \sigma_U(d\alpha).$$

By the relationship between Herglotz functions on the disc and upper half-plane, as discussed in Section 4, we have that

$$\operatorname{Re}(G_{\Phi_A}(z)) = \sigma_U(\{1\})\operatorname{Im}(z) + \int_{-\infty}^{\infty} \operatorname{Re}\left(\frac{1}{i\pi} \frac{1}{t-z}\right) \Sigma_A(dt),$$

or equivalently

$$\begin{aligned} G_{\Phi_A}(z) &= -iz\sigma_U(\{1\}) + \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{tz+1}{t-z} \frac{1}{1+t^2} \Sigma_A(dt) \\ &= -iz\sigma_U(\{1\}) + \int_{-\infty}^{\infty} \frac{tz+1}{i(t-z)} (\sigma_U \circ b)(dt) \\ &= -iz\sigma_U(\{1\}) + \int_{-\infty}^{\infty} \frac{tz+1}{i(t-z)} J^* P_A(dt) J. \end{aligned}$$

In particular if U does not have 1 as an eigenvalue, then Φ_A is uniquely determined by Σ_A . Note that since U is unitary, the projection-valued measure P_U is unital which implies that σ_U is a unital probability measure so that $g_\phi(0) = \mathbb{1}$, and this in turn implies that $\phi(0) = 0$, and that

$$\Phi[A; B](i) = 0,$$

for any $A \in \operatorname{Ext}(B)$.

Remark 8.6. Our definition of the characteristic function $\Phi[A; B]$ of the extension A relative to B is really an equivalent reformulation of the concepts of the Weyl-Titchmarsh function and the Livsic characteristic function of the pair (B, A) [19, 20, 21].

Namely in [19], Donoghue defines the Weyl-Titchmarsh function of a pair (B, A) , where B is a densely defined simple symmetric operator with deficiency indices $(1, 1)$ and $A \in \operatorname{Ext}(B)$ by the formula

$$\begin{aligned} M(B, A)(z) &:= \langle (Az + i)(A - zI)^{-1} g_+, g_+ \rangle \\ &= \int_{-\infty}^{\infty} \frac{tz+1}{t-z} \langle P_A(dt) g_+, g_+ \rangle, \end{aligned}$$

where g_+ is a fixed normalized element in $\operatorname{Ker}(B^* - i)$. In this case where B has indices $(1, 1)$, we can define our isometry $J : \mathbb{C} \rightarrow \operatorname{Ker}(B^* + i)$ in the construction of Γ_A and Ω_A by $J e_1 = g_-$ where $e_1 = 1$ is a trivial orthonormal basis of \mathbb{C} and g_- is a fixed unit element of $\operatorname{Ker}(B^* + i)$. In this case the Herglotz function G_{Φ_A} is just

$$\begin{aligned} G_{\Phi_A}(z) &= -i \int_{-\infty}^{\infty} \frac{tz+1}{(t-z)} J^* P_A(dt) J \\ &= -i \int_{-\infty}^{\infty} \frac{tz+1}{(t-z)} \langle P_A(dt) g_-, g_- \rangle. \end{aligned}$$

This would be simply the Weyl-Titchmarsh function for the pair (B, A) multiplied by $-i$, if we had defined $\Phi[A; B]$ using the deficiency subspace $\operatorname{Ker}(B^* - i)$ instead of $\operatorname{Ker}(B^* + i)$. Namely if we instead define $\check{\sigma}(\Omega) = J_i^* P_U(\Omega) J_i$, \check{g}_U the corresponding Herglotz function on \mathbb{D} , and \check{G}_A the

corresponding Herglotz function on \mathbb{C}_+ , then $\check{G}_A = -iM(B, A)$. Note here that since B is densely defined $U = b(A)$ does not have 1 as an eigenvalue.

In [20], the Livsic function of the pair (A, B) , where B as above has indices $(1, 1)$ is defined to be

$$s(B, A)(z) := \frac{M(z) - i}{M(z) + i}.$$

Again if we had chosen to work with $\text{Ker}(B^* - i)$ instead of $\text{Ker}(B^* + i)$ then we would have that $s(B, A)(z) = \check{\Phi}[A; B](z)$, where $\check{\Phi}[A; B](z)$ is the contractive analytic function corresponding to the Herglotz function $\check{G}_A(z)$.

One can construct a natural bijective map between the sets of functions $\check{\Phi}[A; B]$ and the functions $\Phi[A; B]$ where $\check{\Phi}[A; B]$ is defined using an isometry $J_i : \mathbb{C}^n \rightarrow \text{Ker}(B^* - i)$, and $\Phi[A; B]$ is defined using as isometry $J : \mathbb{C}^n \rightarrow \text{Ker}(B^* + i)$ using the conjugation maps C_B and C_{B_T} described in Section 4. Namely recall that if $B \in \mathcal{S}_n(\mathcal{H})$ has Livsic characteristic function Θ_B , then $B_T \in \mathcal{S}_n(\mathcal{H}_T)$ is a simple symmetric linear transformation with Livsic function Θ_B^T , and there is a pair of anti-unitary maps $C_B : \mathcal{H} \rightarrow \mathcal{H}_T$ and $C_{B_T} : \mathcal{H}_T \rightarrow \mathcal{H}$ such that $C_B^* = C_{B_T}$, $C_B \text{Dom}(B) = \text{Dom}(B_T)$, $C_{B_T} \text{Dom}(B_T) = \text{Dom}(B)$, and $C_B B = B_T C_B$.

There is a bijective correspondence between unitary extensions U of $b(B)$ and positive operator valued measures Q_U on the unit-circle \mathbb{T} which diagonalize $b(B)$, *i.e.* such that for any $f \in \text{Ker}(b(B))^\perp$,

$$b(B)f = \int_{\mathbb{T}} \alpha Q_U(d\alpha).$$

Indeed if U is a unitary extension of $b(B)$, then $Q_U(\Omega) := P_{\mathcal{H}} P_U(\Omega) P_{\mathcal{H}}$ is such a measure diagonalizing $b(B)$, and conversely given such a measure Q , Naimark's dilation theorem provides a unitary extension U on a larger Hilbert space $\mathcal{K} \supset \mathcal{H}$ with the property that $Q(\Omega) := P_{\mathcal{H}} P_U(\Omega) P_{\mathcal{H}}$. One can then check that the map $Q \mapsto \check{Q}$ defined by

$$\check{Q}(\Omega) := C_B Q(\Omega) C_{B_T},$$

is a bijective map from the positive operator-valued measures diagonalizing $b(B)$ to those diagonalizing $b(B_T)$. Since there is a bijection between such measures and extensions $A_T \in \text{Ext}(B_T)$, this constructs a bijection from extensions $A \in \text{Ext}(B)$ to extensions $A_T \in \text{Ext}(B_T)$.

Now let $\{u_j\}, \{v_j\}$ be orthonormal bases of $\text{Ker}(B^* - i)$ and $\text{Ker}(B^* + i)$ respectively, and let $\check{u}_j = C_B u_j$ and $\check{v}_j = C_B v_j$ be corresponding basis elements for $\text{Ker}(B_T^* \pm i)$, and suppose that $J_{\pm i} : \mathbb{C}^n \rightarrow \text{Ker}(B^* \mp i)$ are isometries defined by $J_{-i} e_k = v_k$, $J_i e_k = u_k$, and define $\check{J}_{\pm i}$ similarly. Then $C_B J_{\pm i} = \check{J}_{\pm i}$, and it follows that if

$$\begin{aligned} M(A, B)(z) &:= \sigma_U(\{1\}) + \int_{-\infty}^{\infty} \frac{tz + 1}{t - z} J_i^* P_A(dt) J_i \\ &= J_i^* Q_U(\{1\}) J_i + \int_{-\infty}^{\infty} \frac{tz + 1}{t - z} J_i^* Q_A(dt) J_i, \end{aligned}$$

where $Q_A(\Omega) := P_{\mathcal{H}}P_A(\Omega)P_{\mathcal{H}}$, then this is the suitable generalization of Donoghue's Weyl-Titchmarsh function to the case where B has indices (n, n) and is not necessarily densely defined. Moreover

$$\begin{aligned} M(A, B)(z) &= \check{J}_{-i}^* C_B Q_U(\{1\}) C_{B_T} \check{J}_{-i} + \int_{-\infty}^{\infty} \frac{tz+1}{t-z} \check{J}_{-i}^* C_B Q_A(dt) C_{B_T} \check{J}_{-i} \\ &= \check{J}_{-i} P_{U_T}(\{1\}) \check{J}_{-i} + \int_{-\infty}^{\infty} \frac{tz+1}{t-z} \check{J}_{-i}^* P_{A_T}(dt) C_{B_T} \check{J}_{-i} \\ &= i\Phi[B_T; A_T](z), \end{aligned} \tag{8.8}$$

so that $M(A, B) = i\Phi(B_T; A_T)$.

This relationship between our characteristic function $\Phi[A; B]$ of the extension A relative to B and the Weyl-Titchmarsh function $M(B, A)$ of the pair (B, A) , allows one to translate all of our upcoming results on $\Phi[A; B]$ and its relationship to Θ_B into equivalent statements about $M(B; A)$.

Theorem 8.7. *If $\tilde{\Phi}_A$ is the contractive analytic function with Herglotz function πG_{Φ_A} , then $\mathcal{K}_A = L(\tilde{\Phi}_A)$.*

In particular if $U = b(A)$ does not have 1 as an eigenvalue then \mathcal{K}_A is the space of Cauchy transforms of the positive operator-valued measure $\pi\Sigma_A$.

Proof. Let $\tilde{\Phi} := \tilde{\Phi}_A$. It suffices to show that $K_w(z) = K_w^{\tilde{\Phi}}(z)$ where $K_w(z) = \Omega(z)^* \Omega(w)$ is the reproducing kernel for \mathcal{K}_A . First

$$K_w(z) = \Omega(z)^* \Omega(w) = J^* U_{-i, z}^* U_{-i, w} J,$$

where $U_{-i, z}$ is given by equation (5.2) so that

$$\begin{aligned} K_w(z) &= 4J^* ((i+z)U + (i-z))^{-1} ((\bar{w}-i)U^* - (\bar{w}+i))^{-1} J \\ &= \frac{4\sigma_U(\{1\})}{((i+z) + (i-z))((\bar{w}-i) - (\bar{w}+i))} + \\ &\quad + \frac{4}{\pi} \int_{\mathbb{T} \setminus \{1\}} \frac{1}{(i+z)\alpha + (i-z)} \frac{1}{(\bar{w}-i)\bar{\alpha} - (\bar{w}+i)} \sigma_U(d\alpha) \\ &= \sigma_U(\{1\}) + \frac{1}{\pi^2} \int_{-\infty}^{\infty} \frac{1}{(t-z)(t-\bar{w})} \pi\Sigma_A(dt) \\ &= K_w^{\tilde{\Phi}}(z), \end{aligned}$$

where the last equality follows from equation (4.5) and the definition of $\tilde{\Phi}_A$. \square

Now let us compute the Livsic characteristic function of the operator $\mathfrak{J} := \mathfrak{J}_{\tilde{\Phi}_A} \in \mathcal{S}_n(L(\tilde{\Phi}_A))$ which acts as multiplication by the independent variable in $L(\tilde{\Phi}_A) = \mathcal{K}_A$. We have

$$\begin{aligned} \{u_j := K_{-i} K_{-i}(-i)^{-1/2} e_j\} &\quad \text{orthonormal basis of } \text{Ker}(\mathfrak{J}^* - i), \\ \{v_j := K_i K_i(i)^{-1/2} e_j\} &\quad \text{orthonormal basis of } \text{Ker}(\mathfrak{J}^* + i), \\ \{w_j(z) = K_{\bar{z}} e_j\} &\quad \text{basis of } \text{Ker}(\mathfrak{J}^* - z). \end{aligned}$$

Note that $K_i(i) = K_{-i}(-i) = J^* J = \mathbb{1}$. By Section 6.3, we can compute the Livsic characteristic function of \mathfrak{J} in two ways:

We have that

$$D(z) = [\langle w_j(z), u_k \rangle] = \left[\left\langle K_{\bar{z}} e_j, K_{-i} K_{-i}(-i)^{-1/2} e_k \right\rangle \right] = K_{\bar{z}}(-i),$$

and

$$C(z) = [\langle w_j(z), v_k \rangle] = K_{\bar{z}}(i).$$

Similarly

$$\tilde{D}(z) = [\langle v_j, w_j(\bar{z}) \rangle] = K_i(z),$$

and

$$\tilde{C}(z) = [\langle u_j, w_j(\bar{z}) \rangle] = K_{-i}(z).$$

Livsic's theorem implies that the functions

$$\Lambda_A(z) := b(z)D(z)^{-1}C(z) \quad \text{and} \quad \tilde{\Lambda}_A(z) := b(z)\tilde{D}(z)^{-1}\tilde{C}(z), \quad (8.9)$$

are both contractive and equal (modulo multiplication to the left and right by fixed unitaries) to the Livsic characteristic function $\Theta_{\mathfrak{J}}$ of \mathfrak{J} . Recall that the Livsic characteristic function is only defined up to unitary coincidence, so this means that there are fixed unitary matrices U, V such that

$$U\Lambda_A V = \tilde{\Lambda}_A.$$

Explicitly we have

$$\tilde{\Lambda}_A(z) = b(z)K_i(z)^{-1}K_{-i}(z) \quad \text{and} \quad \Lambda_A(z) = b(z)K_{\bar{z}}(-i)^{-1}K_{\bar{z}}(i). \quad (8.10)$$

Theorem 8.8. *The contractive analytic functions Λ_A and $\tilde{\Lambda}_A$ are both equal to $\Phi_A = \Phi[B; A]$.*

Proof. Since Λ_A is the characteristic function of \mathfrak{J}_{Φ_A} , and since $K_w^{\tilde{\Phi}_A}(z) = \pi K_w^{\Phi_A}(z)$, it follows that

$$\Lambda_A(z) = b(z)K_{\bar{z}}^{\Phi_A}(-i)^{-1}K_{\bar{z}}^{\Phi_A}(i).$$

This shows that Λ_A is the Livsic characteristic function of \mathfrak{J}_{Φ_A} , and Lemma 4.4 of Section 4 implies that Λ_A is the Frostman shift of Φ_A which vanishes at i . However since $\Phi_A(i) = 0$, this Frostman shift is just equal to Φ_A and $\Phi_A = \Lambda_A$.

Now, $\tilde{\Lambda}_A(z) = b(z)K_i(z)^{-1}K_{-i}(z)$. Using that $G_A(\bar{z})^* = -G_A(z)$, one can calculate that

$$\begin{aligned} b(z)K_i(z)^{-1}K_{-i}(z) &= (G_A(z) + G_A(i)^*)^{-1}(G_A(z) - G_A(i)) \\ &= b(z)K_{\bar{z}}(-i)^{-1}K_{\bar{z}}(i) = \Lambda_A(z). \end{aligned}$$

This shows that $\tilde{\Lambda}_A(z) = \Lambda_A(z)$. □

Theorem 8.9. *Given any $A \in \text{Ext}(B)$, we have that $\Phi_A \geq \Theta_B$, i.e. $\Theta_B(z)^{-1}\Phi_A(z)$ is a contractive analytic function in \mathbb{C}_+ .*

Proof. Consider again the symmetric linear transformation \mathfrak{J} which acts as multiplication by z in $\mathcal{L}(\tilde{\Phi}_A) = \mathcal{K}_A$, where $\tilde{\Phi}$ is the contractive analytic function corresponding to the measure $\pi\Sigma_A$. We can construct a canonical model for \mathfrak{J} by choosing $\mathcal{J} := \mathbb{C}^n$ with orthonormal basis $\{e_j\}$ and defining

$$\Gamma(z) := K_z e_j,$$

where $K_z(w)$ is the reproducing kernel for \mathcal{K}_A . If we do this we find that $(\mathcal{K}_A)_\Gamma = \mathcal{K}_A$ and that U_Γ is just the identity on \mathcal{K}_A . Hence it follows from Section 6.4, and in fact from [4], that we can

express the reproducing kernel for \mathcal{K}_A as

$$K_z(z) = \frac{K_i(z)K_i(i)^{-1}K_i(z)^* - |b(z)|^2 K_{-i}(z)K_{-i}(-i)^{-1}K_{-i}(z)^*}{1 - |b(z)|^2}.$$

We can write this as

$$(1 - |b(z)|^2)K_z(z) = \tilde{D}(z)\tilde{D}(z)^* - |b(z)|^2\tilde{C}(z)\tilde{C}(z)^*,$$

where $\Phi_A(z) = \Lambda_A(z) = \tilde{\Lambda}_A(z) = b(z)\tilde{D}(z)^{-1}\tilde{C}(z)$, and $\tilde{D}(z) = K_i(z)$.

Also note that if $k_w(z)$ is the reproducing kernel for \mathcal{H}_A , then for any $z \in \Pi_A^+$ (which is dense in \mathbb{C}_+) we can write

$$(1 - |b(z)|^2)k_z(z) = B(z)B(z)^* - |b(z)|^2 A(z)A(z)^*,$$

where $\Theta_B(z) = b(z)B(z)^{-1}A(z)$ and $B(z) = k_i(z) = \Gamma(z)^*\Gamma(i) = \Gamma(z)^*J = \Omega(z)^*\Omega(i) = K_i(z)$. Hence $B(z) = \tilde{D}(z)$.

Now since $A \in \text{Ext}(B)$, \mathcal{H}_A is isometrically contained in \mathcal{K}_A so that $K_z(z) - k_z(z) \geq 0$. Hence we have that

$$\tilde{D}(z)\tilde{D}(z)^* - |b(z)|^2\tilde{C}(z)\tilde{C}(z)^* \geq \tilde{D}(z)\tilde{D}(z)^* - |b(z)|^2 A(z)A(z)^*. \quad (8.11)$$

so that

$$A(z)A(z)^* \geq \tilde{C}(z)\tilde{C}(z)^*,$$

and hence

$$B^{-1}(z)A(z)A(z)^*B^{-1}(z)^* \geq \tilde{D}(z)^{-1}\tilde{C}(z)\tilde{C}(z)^*(\tilde{D}(z)^*)^{-1}.$$

Since $\tilde{\Lambda}_A(z) = \Lambda_A(z) = \Phi_A(z)$, this shows that

$$\Theta_B(z)\Theta_B(z)^* \geq \Phi_A(z)\Phi_A(z)^*, \quad (8.12)$$

proving the theorem. □

Example 8.10. Consider the finite dimensional partial isometry V :

$$V := \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

Clearly $V \in \mathcal{V}_1(\mathbb{C}^2)$.

Now let

$$U := \begin{pmatrix} 0 & 3/5 & 4/5 \\ 1 & 0 & 0 \\ 0 & 4/5 & -3/5 \end{pmatrix}.$$

This is a unitary matrix acting on \mathbb{C}^3 , and $U|_{\text{Ker}(V)^\perp} = V|_{\text{Ker}(V)^\perp}$ so that $V \subseteq U$ and so if $B := b^{-1}(B) \in \mathcal{S}_1(\mathbb{C}^2)$ then we have that $A := b^{-1}(U) \in \text{Ext}(B)$.

Our goal is to calculate Φ_A and to verify that $\Phi_A \geq \Theta_B$.

First we calculate Θ_B , the characteristic function of $B = b^{-1}(V) = i(1 + V)(1 - V)^{-1}$. We will denote the standard bases of \mathbb{C}^n by $\{e_k\}$. Now

$$\text{Ker}(B^* - i) = \text{Ker}(V) = \bigvee \{e_2\} \quad \text{and} \quad \text{Ker}(B^* + i) = \text{Ran}(V)^\perp = \bigvee \{e_1\}.$$

Note that to avoid writing column vectors we will write $(a, b)^T$ to denote the transpose of the row vector (a, b) , and sometimes we will omit the T in our calculations.

To calculate the Livsic characteristic function we also need to determine $\text{Ker}(B^* - z)$. First we calculate $\text{Ran}(B - z)$:

$$\text{Ran}(B - z) = i(1 + V)\text{Ker}(V)^\perp - z(1 - V)\text{Ker}(V)^\perp = ((i - z) + (i + z)V)\text{Ker}(V)^\perp.$$

Since $\text{Ker}(V)^\perp$ is spanned by e_1 and $Ve_1 = e_2$, we get that $\text{Ran}(B - z)$ is spanned by

$$((i - z), (i + z))^T.$$

It follows that if $(c, d)^T \in \text{Ker}(B^* - \bar{z})$, that

$$(\bar{c}, \bar{d}) \cdot (i - z, i + z) = 0,$$

and this shows that $\text{Ker}(B^* - z)$ is spanned by

$$w(z) := (z - i, z + i)^T.$$

Finally

$$\Theta_B(z) = b(z) \frac{(w(z), e_1)}{(w(z), e_2)} = \left(\frac{z - i}{z + i} \right)^2.$$

To calculate Φ_A , we first need to calculate the projection-valued measure of U . We begin by calculating the eigenvalues and eigenvectors of U : We have

$$\det(\lambda - U) = \lambda^3 + 3/5\lambda^2 - 3/5\lambda - 1 = (\lambda - \lambda_1)(\lambda - \lambda_2)(\lambda - \lambda_3),$$

where $\lambda_1 = 1$, $\lambda_2 := -4/5 + i3/5 =: \beta$ and $\lambda_3 = \bar{\lambda}_2 = \bar{\beta}$. A normalized eigenvector for $\lambda_1 = 1$ is:

$$\hat{b}_1 := (2/3, 2/3, 1/3)^T,$$

and (non-normalized) eigenvectors for $\beta, \bar{\beta}$ are:

$$\vec{b}_2 = (1, \beta, 5/4(\beta^2 - 3/5)\beta)^T,$$

and

$$\vec{b}_3 = (1, \bar{\beta}, 5/4(\bar{\beta}^2 - 3/5)\bar{\beta})^T.$$

It follows that the projection-valued measure of U is given by

$$P_U = \sum_{i=1}^3 \left(\cdot, \hat{b}_i \right) \hat{b}_i \delta_{\lambda_i},$$

where the δ_{λ_i} are Dirac point measures of weight one at the points λ_i , and the \hat{b}_i are normalized eigenvectors to the eigenvalues λ_i . Now the scalar measure σ_U which determines ϕ_U , where $\Phi_A = \phi_U \circ b$, is given by

$$\sigma_U(\Omega) = \langle v, P_U(\Omega)v \rangle,$$

where $v = e_1$ is a unit vector spanning $\text{Ran}(V)^\perp = \text{Ker}(B^* + i)$. Hence

$$\sigma_U(\Omega) = \sum_{k=1}^3 | \left(e_1, \hat{b}_k \right) |^2 \delta_{\lambda_k}.$$

Now $(e_1, \hat{b}_1) = 2/3$, and since $\vec{b}_2 = C\vec{b}_3$ is the component-wise complex conjugate of \vec{b}_3 , it follows that $|(e_1, \hat{b}_2)|^2 = |(e_1, \hat{b}_3)|^2 =: a$. Finally since P_U is unital, σ_U must be a probability measure:

$$1 = \sum_{k=1}^3 |(e_1, \hat{b}_k)|^2 = 4/9 + 2a,$$

proving that $a = 5/18$. In conclusion,

$$\sigma_U = \frac{4}{9}\delta_1 + \frac{5}{18}\delta_\beta + \frac{5}{18}\delta_{\bar{\beta}},$$

where $\beta = -4/5 + i3/5$. It follows that

$$g_{\phi_U}(w) = \int_{\mathbb{T}} \frac{\alpha + w}{\alpha - w} \sigma_U(d\alpha),$$

$$G_{\Phi_A}(z) = -i\sigma_U(\{1\})z + \int_{-\infty}^{\infty} \left(\frac{zt+1}{i(t-z)} \right) \tilde{\sigma}_U(dt),$$

where $\tilde{\sigma}_U := \sigma_U \circ b$. An easy calculation shows that $b^{-1}(\beta) = 1/3$ and $b^{-1}(\bar{\beta}) = -1/3$, and so it follows that

$$G_{\Phi_A}(z) = -i\frac{4}{9}z + \frac{5}{18} \frac{z/3+1}{1/3-z} + \frac{5}{18} \frac{z/3-1}{1/3+z}.$$

Notice that $G_{\Phi_A}(i) = 1$ as expected. Hence

$$\begin{aligned} \Phi_A(z) &= \frac{\left(\frac{4}{9} + \frac{5}{18} \frac{z+3}{1-3z} + \frac{5}{18} \frac{z-3}{1+3z} \right) - i}{\left(\frac{4}{9} + \frac{5}{18} \frac{z+3}{1-3z} + \frac{5}{18} \frac{z-3}{1+3z} \right) + i} \\ &= \frac{z(1-3z)(1+3z) + \frac{5}{8}((z+3)(1+3z) + (z-3)(1-3z)) - i\frac{9}{4}(1-3z)(1+3z)}{z(1-3z)(1+3z) + \frac{5}{8}((z+3)(1+3z) + (z-3)(1-3z)) + i\frac{9}{4}(1-3z)(1+3z)}. \end{aligned}$$

The numerator simplifies to

$$n(z) = -9z^3 + i\frac{81}{4}z^2 + \frac{27}{2}z - i\frac{9}{4}.$$

Let $p(z) = \frac{n(z)}{-9} = z^3 - i\frac{9}{4}z^2 - \frac{3}{2}z + \frac{i}{4}$. It follows that $\Phi_A(z)$ is the product of three Blaschke factors, one for each of the roots of $p(z)$. It is easy to calculate that $p(z)$ factors as $p(z) = (z-i)^2(z - \frac{i}{4})$, and so (up to a unimodular constant),

$$\Phi_A(z) = \frac{(z-i)^2(z-i/4)}{(z+i)^2(z+i/4)},$$

which is indeed greater or equal to

$$\Theta_B(z) = \left(\frac{z-i}{z+i} \right)^2.$$

Definition 8.11. We say that $A_1 \sim A_2$ if $\Phi_{A_1} = \Phi_{A_2}$. This is clearly an equivalence relation. Let $\text{ext}(B) := \text{Ext}(B)/\sim$. That is $\text{ext}(B)$ is the set of all \sim equivalence classes of $\text{Ext}(B)$.

Suppose that $A_1, A_2 \in \text{Ext}(B)$ are such that $A_k = b^{-1}(U_k)$ for $U_k \in \text{Ext}(b(B))$ which do not have 1 as an eigenvalue. Then:

Theorem 8.12. $A_1 \sim A_2$ if and only if $A_1 \simeq A_2$ via a unitary U whose restriction to \mathcal{H} is the identity.

The above result is easily extended to include the exceptional case where one (or both) A_1, A_2 are defined using $U_1, U_2 \in \text{Ext}(b(B))$ where 1 is an eigenvalue of either U_1 or U_2 . Namely the statement of the theorem becomes: Suppose $A_1, A_2 \in \text{Ext}(B)$ are defined using $U_1, U_2 \in \text{Ext}(b(B))$. Then $A_1 \sim A_2$ if and only if $U_1 \simeq U_2$ via a unitary U which fixes \mathcal{H} .

Proof. If such a unitary U exists then

$$\Sigma_1(\Omega) := \Sigma_{A_1}(\Omega) = \int_{\Omega} \pi(1 + t^2) J^* P_1(dt) J,$$

and

$$\begin{aligned} J^* P_1(dt) J &= J^* U^* U P_1(dt) J \\ &= J^* U^* P_2(dt) U J \\ &= J^* P_2(dt) J, \end{aligned} \tag{8.13}$$

since $UJ = J$ as $U|_{\mathcal{H}} = \mathbb{1}_{\mathcal{H}}$. It follows that $\Sigma_1 = \Sigma_2$ which implies $\Phi_1 = \Phi_2$.

Conversely suppose that $\Phi_1 = \Phi_{A_1} = \Phi_{A_2} = \Phi_2$. It follows then that $\Sigma_1 = \Sigma_2$ so that

$$J^* P_1(\Omega) J = J^* P_2(\Omega) J.$$

It follows that for any bounded Borel function g on \mathbb{R} ,

$$J^* g(A_1) J = J^* g(A_2) J.$$

Since $\text{Ker}(B^* + i) = J\mathbb{C}^n$ is cyclic for A_j (by Theorem 7.3 since Θ_B is inner), for $j = 1, 2$, it follows that we can define a unitary $U : \mathcal{K}_1 \rightarrow \mathcal{K}_2$ as follows. Let $\{v_k = J e_k\}$ be an orthonormal basis of $P_{-i}\mathcal{H}$. Any $f \in \mathcal{K}_1$ can be written

$$f = f_1(A_1)v_1 + \dots + f_n(A_1)v_n,$$

and define

$$Uf = f_1(A_2)v_1 + \dots + f_n(A_2)v_n.$$

This is isometric because

$$\begin{aligned} \langle f_k(A_1)v_k, f_j(A_1)v_j \rangle &= \langle J^* \overline{f_j}(A_1) f_k(A_1) J e_k, e_j \rangle \\ &= \langle J^* \overline{f_j}(A_2) f_k(A_2) J e_k, e_j \rangle \\ &= \langle U f_k(A_1)v_k, U f_j(A_1)v_j \rangle. \end{aligned} \tag{8.14}$$

The map U is also onto because $\text{Ker}(B^* + i)$ is cyclic for A_1 and A_2 .

□

Remark 8.13. Suppose that $A \in \text{Ext}_U(B)$, which is to say that there is an isometry $U : \mathcal{H} \rightarrow \mathcal{K}$ such that $A \in \text{Ext}(UBU^*)$. In this case we define $\Phi_A := \Phi[A; UBU^*]$.

Note that if $A \in \text{Ext}_U(B)$ has characteristic function Φ_A , then there is a corresponding $A' \in \text{Ext}(B)$ such that $\Phi_{A'} = \Phi_A$. This follows from Naimark's dilation theorem [16, Theorem 4.6].

Indeed if $A \in \text{Ext}_U(B)$ so that $A \in \text{Ext}(UBU^*)$ for some isometry $U : \mathcal{H} \rightarrow \mathcal{K}$ then

$$Q(\Omega) := P_{\mathcal{H}} U^* P_A(\Omega) U P_{\mathcal{H}},$$

is a positive operator-valued measure acting on \mathcal{H} . Assume for now that A is defined using a $W \in \text{Ext}(Ub(B)U^*)$ which does not have 1 as an eigenvalue so that $A = b^{-1}(W)$.

Since $A = b^{-1}(W)$ and $1 \notin \sigma_p(W)$, A is a densely defined self-adjoint operator and $P_A(\mathbb{R}) := \chi_{\mathbb{R}}(A) = \mathbb{1}_{\mathcal{K}}$, as otherwise $P_A(\mathbb{R})\mathcal{K}$ is a non-trivial reducing subspace for A which contains \mathcal{H} . In other words the projection-valued measure of A is unital.

By Naimark's dilation theorem there is a larger Hilbert space $\mathcal{K}' \supset \mathcal{H}$ and a unital projection-valued measure $P(\Omega)$ acting on \mathcal{K}' such that the compression

$$P_{\mathcal{H}}P(\Omega)P_{\mathcal{H}} = Q(\Omega),$$

for any Borel set Ω . This projection-valued measure P is called a dilation of Q , and it can be chosen to be minimal in the sense that $\mathcal{K}' = \bigvee P(\Omega)\mathcal{H}$. If A' is the self-adjoint operator corresponding to this projection valued measure,

$$A' := \int_{-\infty}^{\infty} tP(dt),$$

then it follows that $A' \in \text{Ext}(B)$. It is also clear that by definition, $\Phi_A = \Phi_{A'}$.

If A is defined using $W \in \text{Ext}(Ub(B)U^*)$ with $1 \in \sigma_p(U)$, define $Q(\Omega) = P_{\mathcal{H}}P_U(\Omega)P_{\mathcal{H}}$, a unital positive operator-valued measure (POVM) on the unit circle. Again apply Naimark's dilation theorem to obtain a unitary operator U' on $\mathcal{K}' \supset \mathcal{H}$. As before it follows that if $A' \in \text{Ext}(B)$ is defined using $U' \in \text{Ext}(b(B))$, that $\Phi_{A'} = \Phi_A$.

Theorem 8.14. *The map $A \in \text{ext}(B) \mapsto \Phi_A$ is a bijection onto the set of all contractive analytic functions Φ_A which are greater or equal to Θ_B .*

This needs some setup: Given $B \in \mathcal{S}_n(\mathcal{H})$ with characteristic function Θ_B let $V := b(B)(1 - P_i)$, the partial isometric extension of $b(B)$, and define $\theta_V := \Theta_B \circ b^{-1}$, a contractive analytic function on the unit disc, \mathbb{D} . Here, as before P_i projects onto $\text{Ker}(B^* - i)$.

Recall that the Alexandrov-Clark measures for θ_V are defined as the $n \times n$ matrix-valued measures δ_U for any $U \in \mathcal{U}(n)$ (the group of $n \times n$ unitary matrices) associated with the Herglotz functions

$$g_U := \frac{1 + \theta_V U^*}{1 - \theta_V U^*},$$

via the Herglotz representation theorem for the unit disk *i.e.*

$$\text{Re}(g_U(z)) = \int_{\mathbb{T}} \text{Re}\left(\frac{\alpha + z}{\alpha - z}\right) \delta_U(d\alpha).$$

Let $G_U := g_U \circ b$ be the corresponding Herglotz function on \mathbb{C}_+ . We define the Alexandrov-Clark measures of Θ_B to be the measures Δ_U on \mathbb{R} such that

$$\text{Re}(G_U(z)) = \delta_U(\{1\})\text{Im}(z) + \int_{-\infty}^{\infty} \text{Re}\left(\frac{1}{i\pi} \frac{1}{t - z}\right) \Delta_U(dt).$$

Recall that as discussed in Section 4 (see equation (4.1)) we have that

$$\Delta_U(\Omega) := \int_{\Omega} \pi(1 + t^2)(\delta_U \circ b)(dt),$$

where $(\delta_U \circ b)(\Omega) = \delta_U(b(\Omega))$ and $b(z) = \frac{z-i}{z+i}$, $b : \mathbb{R} \rightarrow \mathbb{T} \setminus \{1\}$.

Now let Z denote the unitary operator of multiplication by z in $L^2_\theta(\mathbb{T})$ (the L^2 space of vector-valued functions on \mathbb{T} which are square integrable with respect to the measure δ_1).

Let $\{b_j^-(z) = e_j\}$ be a basis for the constant functions in L^2_θ . Since $\Theta(i) = 0 = \theta(0)$, it follows that this is an orthonormal basis. Similarly define $b_j^+(z) := \frac{1}{z}e_j$. For any $A \in \mathbb{C}^{n \times n}$ let

$$Z(A) := Z + P_-(\tilde{A} - 1)P_-Z,$$

where P_- projects onto the closed span of the b_j^- , and $\tilde{A} = j^*Aj$ where j is an isomorphism defined by $j e_k = b_k^-$ which takes \mathbb{C}^n onto the range of P_- . Then as shown in [8] $Z(0)$ has Livsic characteristic function θ_V , and so it follows that there is a unitary transformation $W : \mathcal{H} \rightarrow L^2_\theta$ that implements the equivalences $Z(0) \simeq V = b(B)(1 - P_i)$, and $Z(U) \simeq V(U)$ for any $U \in \mathcal{U}(n)$, and such that $W : \text{Ker}(B^* - i) = \text{Ker}(V) \rightarrow \text{Ker}(Z(0)) = \bigvee b_j^-$ sends $u_j \mapsto b_j^-$ [8, 2], where $\{u_j\}$ is an orthonormal basis of $\text{Ker}(B^* - i)$.

Moreover the results of [2] show that

$$\delta_U(\Omega) = [\langle \chi_\Omega(Z(U))b_i^-, b_j^- \rangle].$$

Using the fact that $G_U = g_U \circ b$, and the relationship between Herglotz functions and measures on the upper half-plane and the disk as described in Section 4, it follows that

$$\text{Re}(G_U(w)) = \delta_U(\{1\})\text{Im}(w) + \int_{-\infty}^{\infty} \text{Re}\left(\frac{1}{i\pi} \frac{1}{t - z}\right) \pi(1 + t^2) \tilde{\Delta}_U(dt),$$

where $\tilde{\Delta}_U := \delta_U \circ b$ so that

$$\begin{aligned} \tilde{\Delta}_U(\Omega) &= [\langle \chi_{b(\Omega)}(Z_U)b_i^+, b_j^+ \rangle] \\ &= [\langle \chi_{b(\Omega)}(b(B(U)))u_i, u_j \rangle] \\ &= [\langle \chi_\Omega(B(U))u_i, u_j \rangle], \end{aligned} \tag{8.15}$$

and

$$\delta_U(\{1\}) = [\langle \chi_{\{1\}}(Z(U))b_i^+, b_j^+ \rangle] = [\langle \chi_{\{1\}}(b(B(U)))u_i, u_j \rangle].$$

Theorem 8.15. *For any $U \in \mathcal{U}(n)$, $\Phi_{B(U)} = U^* \Theta_B$.*

Proof. Let $B_T \in \mathcal{S}_n(\mathcal{H}_T)$ be a symmetric linear transformation with characteristic function Θ_B^T , and let $\{\tilde{u}_j\}$, $\{\tilde{v}_j\}$ be orthonormal bases of $\text{Ker}(B_T^* - i)$ and $\text{Ker}(B_T^* + i)$, respectively.

By Corollary 4.9, there is a conjugation $C_T := C_{B_T} : \mathcal{H}_T \rightarrow \mathcal{H}$ which intertwines B_T and B . Let $\{u_k\}$, $\{v_k\}$ be the orthonormal bases of $\text{Ker}(B^* - i)$ and $\text{Ker}(B^* + i)$ respectively given by $C_T \tilde{u}_j = v_j$ and $C_T \tilde{v}_j = u_j$. Further recall that $C_T^* = C_B$ is a conjugation intertwining B and B_T so that $C_B v_j = \tilde{u}_j$ and $C_B u_j = \tilde{v}_j$. Also define $J : \mathbb{C}^n \rightarrow \text{Ker}(B^* - i)$ by $J e_k = v_k$, for some orthonormal basis $\{e_k\}$ of \mathbb{C}^n .

Let V and V_T be the partial isometric extensions of the Cayley transforms of B , and B_T . Given any $U \in \mathcal{U}(n)$, let

$$V(U) := V + \hat{U} := V + \sum_{i,j} U_{ij} \langle \cdot, u_i \rangle v_j.$$

The set of all $V(U)$, for $U \in \mathcal{U}(n)$ is the set of all canonical unitary extensions of V , and the set of all $B(U) := b^{-1}(V(U))$ is the set of all canonical self-adjoint extensions of B . Similarly define

$$V_T(U) := V_T + \tilde{U} := V_T + \sum_{i,j} U_{ij} \langle \cdot, \tilde{u}_i \rangle \tilde{v}_j.$$

Consider the self-adjoint extension $B_T(U) = b^{-1}(V_T(U))$, where V_T is the partial isometric extension of $b(B_T)$. Then

$$\text{Dom}(B_T(U)) = \text{Ran}(1 - V_T(U)) = \text{Dom}(B_T) + (1 - \tilde{U}) \tilde{S}_{-i},$$

where $\tilde{S}_{\pm i} = \tilde{P}_{\pm i} \mathcal{H}$, and $\tilde{P}_{\pm i}$ are the projections onto $\text{Ker}(B_T^* \pm i)$. Similarly define $S_{\pm i}$ and $P_{\pm i}$. As above, \tilde{U} is defined by

$$\tilde{U} = \sum_{i,j} U_{ij} \langle \cdot, \tilde{u}_i \rangle \tilde{v}_j : \tilde{S}_i \rightarrow \tilde{S}_{-i}.$$

Given any $g \in \text{Dom}(B_T(U))$, it follows that there is some $\tilde{f} = \sum \langle \tilde{f}, \tilde{u}_i \rangle \tilde{u}_i \in \tilde{S}_i$ and $g_T \in \text{Dom}(B_T)$ such that

$$\begin{aligned} g &= g_T + \sum \langle \tilde{f}, \tilde{u}_i \rangle \tilde{u}_i - \sum U_{ij} \langle \tilde{f}, \tilde{u}_i \rangle \tilde{v}_j \\ &= g_T + \tilde{f} - \tilde{U} \tilde{f}, \end{aligned}$$

so that

$$B_T(U)g = B_T g_T + i\tilde{f} + i\tilde{U}\tilde{f}.$$

Now $C_T g_T = g_B \in \text{Dom}(B)$, and

$$\begin{aligned} C_T g &= g_B + \sum \overline{\langle \tilde{f}, \tilde{u}_i \rangle} v_i - \sum \overline{U_{ij}} \overline{\langle \tilde{f}, \tilde{u}_i \rangle} u_j \\ &= g_B + f - \hat{W} f, \end{aligned} \tag{8.16}$$

where $C_T \tilde{f} = f := \sum \overline{\langle \tilde{f}, \tilde{u}_i \rangle} v_i \in S_{-i}$ and

$$\hat{W} = \sum_{i,j} \overline{U_{ij}} \langle \cdot, v_i \rangle u_j.$$

Comparing this to

$$\hat{U}^* = \sum_{i,j} \overline{U_{ji}} \langle \cdot, v_i \rangle u_j,$$

we see that $\hat{W} = \widehat{U^T}^*$

Now if $R \in \mathcal{U}(n)$ then $b(B(R))^* = V^* + \hat{R}^*$ and if $b^\dagger(z) = \frac{z+i}{z-i}$ then its inverse with respect to composition is $b^{-1}(z)^\dagger = -i \frac{1+z}{1-z}$, so that we also have that $\text{Dom}(B(R)) = \text{Ran}(1 - V(R)^*)$. It follows that

$$C_T g = g_B + f - \widehat{U^T}^* f \in \text{Dom}(B(U^T)),$$

and

$$B(U^T)C_T g = B g_B - i f - i \widehat{U^T}^* f,$$

while

$$C_T B_T(U)g = C_T B_T g_T + C_T(i\tilde{f} + i\tilde{U}\tilde{f}) = B(U^T)C_T g,$$

and this proves that

$$C_T B_T(U) = B(U^T) C_T. \quad (8.17)$$

It further follows that

$$C_T V_T(U) = V(U^T)^* C_T.$$

Now let δ_U be the Alexandrov-Clark measure associated with the Herglotz functions

$$g_U(z) := \frac{1 + \theta^T U^*}{1 - \theta^T U^*},$$

where $\theta^T := \Theta^T \circ b$, and as before let $\tilde{\Delta}_U := \delta_U \circ b^{-1}$. As discussed before this proof, the results of [2] show that

$$\tilde{\Delta}_U(\Omega) = [\langle \chi_\Omega(B_T(U)) \tilde{u}_i, \tilde{u}_j \rangle],$$

so that

$$\begin{aligned} \tilde{\Delta}_U(\Omega) &= [\langle C_T \tilde{u}_j, C_T \chi_\Omega(B_T(U)) \tilde{u}_i \rangle] \\ &= [\langle u_j, \chi_\Omega(B(U^T)) u_i \rangle] \\ &= (J^* P_{B(U^T)}(\Omega) J)^T. \end{aligned}$$

Similarly,

$$\begin{aligned} \delta_U(\{1\}) &= [\langle C_B C_T \chi_{\{1\}}(V_T(U)) \tilde{u}_i, \tilde{u}_j \rangle] \\ &= [\langle v_j, \chi_{\{1\}}(V(U^T)^*) v_i \rangle] \\ &= [\langle v_j, \chi_{\{1\}}(V(U^T)) v_i \rangle] \\ &= (J^* P_{V(U^T)}(\{1\}) J)^T. \end{aligned} \quad (8.18)$$

In conclusion we have that if $\Phi := \Phi_{B(U^T)}$, that $G_\Phi^T = G_U$, so that

$$G_\Phi = G_U^T = \frac{1 + (U^*)^T \Theta_B}{1 - (U^*)^T \Theta_B}.$$

This proves that $\Phi_{B(U^T)} = (U^T)^* \Theta_B$, or equivalently that $\Phi_{B(U)} = U^* \Theta_B$. \square

Proof. (of Theorem 8.14)

This map is automatically injective by the definition of $\text{ext}(B)$. To show that it is surjective, let Φ be a contractive analytic function such that $\Phi \geq \Theta_B$, i.e. $\Theta_B^{-1} \Phi$ is a contractive analytic function. Let $\Theta := \Theta_B$.

Now we have $B \simeq \mathfrak{Z}_\Theta$ acting in $\mathbf{L}(\Theta)$, and by Corollary 4.5, $\mathfrak{Z}_\Theta \lesssim \mathfrak{Z}_\Phi$. Furthermore by Theorem 8.15 we have that there is a canonical self-adjoint extension A of \mathfrak{Z}_Φ whose characteristic function $\Phi_A = \Phi[A; \mathfrak{Z}_\Phi]$ relative to \mathfrak{Z}_Φ is Φ . Moreover one can see from Example 4.6 that the isometry $V : \mathbf{L}(\Theta) \rightarrow \mathbf{L}(\Phi)$ which obeys $V \mathfrak{Z}_\Theta \subset \mathfrak{Z}_\Phi V$ also satisfies $V P_{-i} = Q_{-i} V$ and $V^* V P_{-i} = P_{-i}$ where P_{-i} projects onto $\text{Ker}(\mathfrak{Z}_\Theta^* + i)$ while Q_{-i} projects onto $\text{Ker}(\mathfrak{Z}_\Phi^* + i)$. To see this note that since $\Theta(i) = 0 = \Phi(i)$ that

$$K_i^\Theta(z) = \frac{2}{1 - \Theta(z)} \frac{i}{\pi} \frac{1}{z + i} \quad \text{and} \quad K_i^\Phi(z) = \frac{2}{1 - \Phi(z)} \frac{i}{\pi} \frac{1}{z + i}.$$

Observe that

$$V_1(z) = \frac{1 - \Theta(z)}{2},$$

is an isometry of $L(\Theta)$ onto K_Θ^2 , that K_Θ^2 is isometrically contained in K_Φ^2 (since Θ is inner), and that multiplication by

$$V_2(z) := \frac{2}{1 - \Phi(z)},$$

is an isometry of K_Φ^2 into $L(\Phi)$. Since V acts as multiplication by $V(z) = V_2(z)V_1(z)$, it is an isometry that obeys $VK_i^\Theta \vec{v} = K_i^\Phi \vec{v}$ for any $\vec{v} \in \mathbb{C}^n$.

It follows that the isometry $V : L(\Theta) \rightarrow L(\Phi)$ obeys $V\text{Ker}(\mathfrak{Z}_\Theta^* + i) = \text{Ker}(\mathfrak{Z}_\Phi^* + i)$. This shows that the characteristic function $\Phi_A = \Phi_A[A; \mathfrak{Z}_\Phi] = \Phi$ of A with respect to \mathfrak{Z}_Φ is the same as the characteristic function Φ_A of $A \in \text{Ext}_U(B)$ with respect to B . By Remark 8.13, there is an $A' \in \text{Ext}(B)$ with $\Phi_{A'} = \Phi_A = \Phi$.

Putting it all together we have that

$$B \simeq \mathfrak{Z}_{\Theta_B} \lesssim \mathfrak{Z}_\Phi,$$

so that $B \lesssim \mathfrak{Z}_\Phi$, $A' \in \text{Ext}(B)$ and $\Phi_{A'} = \Phi \geq \Theta_B$. This proves surjectivity. \square

9. PARTIAL ORDER CALCULATIONS

In this section we study the partial order \lesssim on symmetric linear transformations described in the introduction:

Definition 9.1. Given $B_1, B_2 \in \mathcal{S}$ we say that $B_1 \lesssim B_2$ if $B_1 \simeq B'_1 \subset B_2$. Recall here \simeq denotes unitary equivalence.

We assume in this section that $n < \infty$, and under this assumption, it is not difficult to verify that \lesssim is indeed a partial order on the unitary equivalence classes of \mathcal{S} (see [22]). Also, using the Cayley transform, this also defines a partial order on \mathcal{V} . Namely, given $V_1, V_2 \in \mathcal{V}$, $V_1 \lesssim V_2$ if and only if $V_1 \simeq V'_1 \subseteq V_2$, where recall that $V'_1 \subseteq V_2$ means that $V_2|_{\text{Ker}(V'_1)^\perp} = V'_1|_{\text{Ker}(V'_1)^\perp}$. This is the same, modulo unitary equivalence as the partial order defined on partial isometries by Halmos and McLaughlin in [6]. That is, they define $V_1 \leq V_2$ if $V_1 \subseteq V_2$.

The main goal of this section is, given $B_1, B_2 \in \mathcal{S}$ with $\Theta_1 := \Theta_{B_1}$ inner, to provide necessary and sufficient conditions on the characteristic function $\Theta_2 := \Theta_{B_2}$ of B_2 so that $B_1 \lesssim B_2$.

Let $B_1 \in \mathcal{S}_m(\mathcal{H}_1)$ and $B_2 \in \mathcal{S}_n(\mathcal{H}_2)$ be symmetric linear transformations, and suppose that $B_1 \lesssim B_2$. As always in this paper we assume that Θ_1 is inner.

Remark 9.2. Let Σ_2 be the Herglotz measure of Θ_2 . For now we assume that the Herglotz measure σ_2 of $\theta_2 := \Theta_2 \circ b^{-1}$ is such that $\sigma_2(\{1\}) = 0$. Recall from Section 4 that this implies that $W_{\Theta_2} : L_{\Sigma_2}^2 \rightarrow L(\Theta_2)$ is an onto isometry so that $B_2 \simeq M_{\Sigma_2}$. This is the case, in particular, when B_2 is densely defined.

Let $\Sigma := \pi\Sigma_2$ where Σ_2 is the Herglotz measure on \mathbb{R} corresponding to Θ_2 . By Remark 9.2, we can and do assume that $B_2 = M_{\Sigma}$. Recall here that M_{Σ} is the symmetric operator of multiplication by the independent variable in L_{Σ}^2 , where L_{Σ}^2 is the Hilbert space of column vector-valued functions

f which are square integrable with respect to Σ , *i.e.* if $f, g \in L_\Sigma^2$ then

$$\langle f, g \rangle_\Sigma = \int_{-\infty}^{\infty} (\Sigma(dt)f(t), g(t))_{\mathbb{C}^n}.$$

Let $\{e_k\}$ be the standard basis of \mathbb{C}^n , and let $\{v_k\}_{k=1}^n$ be a fixed orthonormal basis of $\text{Ker}(B_2^* + i)$. Define an isomorphism $J : \mathbb{C}^n \rightarrow \text{Ker}(B_2^* + i)$ by $Je_k = v_k$. By our previous result, Theorem 8.15, on Alexandrov-Clark measures, there is a canonical $\mathcal{A} \in \text{Ext}(B_2)$ such that

$$\Phi[\mathcal{A}; B_2] = \Theta_2,$$

and

$$\Sigma(\Omega) = \int_{\Omega} \pi^2(1+t^2)J^*P_{\mathcal{A}}(dt)J.$$

Since we assume that $B_2 = M_\Sigma$ it actually follows that $\mathcal{A} = M^\Sigma$, the self-adjoint operator of multiplication by t in L_Σ^2 .

Remark 9.3. We can further choose

$$v_k := \frac{i}{\pi} \frac{1}{t+i} e_k,$$

this follows because if $\tilde{\Phi}$ is the contractive analytic function corresponding to Σ , then the deBranges-Cauchy transform isometry,

$$W : L_\Sigma^2 \rightarrow \mathbf{L}(\tilde{\Phi}),$$

is onto and acts as

$$Wh(z) = \frac{1}{i\pi} \int_{-\infty}^{\infty} \frac{\overline{1}}{\pi(t-\bar{z})} \Sigma(dt)h(t),$$

and the e_j -point evaluation vector at $z = i$ in $\mathbf{L}(\tilde{\Phi})$ is

$$K_i(z)e_j = \int_{-\infty}^{\infty} \frac{i}{\pi(t+i)} \frac{\overline{i}}{\pi(t-\bar{z})} \Sigma(dt)e_j = Wv_j(z).$$

Since K_ie_j spans $\text{Ker}(\mathfrak{Z}_\Phi^* + i)$, the $W^*K_ie_j = v_j$ span $\text{Ker}(M_\Sigma^* + i)$. Moreover this choice of v_k defines an orthonormal basis since $\Theta_2(i) = 0$ implies that

$$\begin{aligned} \mathbb{1} &= \text{Re}(B_{\Theta_2}(i)) = \int_{-\infty}^{\infty} \text{Re}\left(\frac{1}{i\pi} \frac{1}{t-i}\right) \Sigma_2(dt) \\ &= \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{1+t^2} \Sigma_2(dt) = \frac{1}{\pi^2} \int_{-\infty}^{\infty} \frac{1}{1+t^2} \Sigma(dt). \end{aligned}$$

It follows from this formula that $\langle v_k, v_j \rangle = \delta_{kj}$.

We are also free to assume that $B_1 \subset B_2 = M_\Sigma$ so that $B_1 \in \mathcal{S}_m(S)$ where $S \subset L_\Sigma^2$. Let A be the restriction of $\mathcal{A} = M^\Sigma$ to the intersection of its domain with its smallest reducing subspace containing S . Then $A \in \text{Ext}(B_1)$. Let $\{\tilde{v}_k\}_{k=1}^m$ be an orthonormal basis of $\text{Ker}(B_1^* + i)$, and let $\tilde{J} : \mathbb{C}^m \rightarrow \text{Ker}(B_1^* + i)$ be an isomorphism defined by $\tilde{J}e_k = \tilde{v}_k$. Then if we define

$$\tilde{\Sigma}'(\Omega) := \int_{\Omega} \pi(1+t^2)\tilde{J}^*P_A(dt)\tilde{J},$$

then we have that $\Phi := \Phi[A; B_1]$ is the contractive analytic function corresponding to $\tilde{\Sigma}'$ and we define $\tilde{\Sigma} = \pi\tilde{\Sigma}'$. Now since $\{v_k\}$ is a cyclic set for $M^\Sigma = \mathcal{A}$, we have that

$$\tilde{v}_j = D_{j1}(\mathcal{A})v_1 + \dots + D_{jn}(\mathcal{A})v_n, \quad 1 \leq j \leq m \quad (9.1)$$

for certain functions D_{jk} where $1 \leq j \leq m$ and $1 \leq k \leq n$ and $\frac{1}{t+i}(D_{j1}, \dots, D_{jn})^T \in L_\Sigma^2$ for $1 \leq j \leq m$. Here the superscript T denotes transpose (we view elements of L_Σ^2 as column vector functions).

Now if $f, g \in L_\Sigma^2$, then it follows that

$$\begin{aligned} \langle f, g \rangle_{\tilde{\Sigma}} &= \int_{-\infty}^{\infty} \left(\tilde{\Sigma}(dt)f(t), g(t) \right)_{\mathbb{C}^n} \\ &= \int_{-\infty}^{\infty} \overline{(g_1(t), \dots, g_n(t))} \begin{pmatrix} \tilde{\Sigma}(dt)e_1, e_1 & \cdots & \tilde{\Sigma}(dt)e_n, e_1 \\ \vdots & \ddots & \vdots \\ \tilde{\Sigma}(dt)e_1, e_n & \cdots & \tilde{\Sigma}(dt)e_n, e_n \end{pmatrix} \begin{pmatrix} f_1(t) \\ \vdots \\ f_n(t) \end{pmatrix}. \end{aligned} \quad (9.2)$$

Hence we have that

$$\tilde{\Sigma}(\Omega) = \begin{pmatrix} \langle P_A(\Omega)\tilde{v}_1, \tilde{v}_1 \rangle & \cdots & \langle P_A(\Omega)\tilde{v}_m, \tilde{v}_1 \rangle \\ \vdots & \ddots & \vdots \\ \langle P_A(\Omega)\tilde{v}_1, \tilde{v}_m \rangle & \cdots & \langle P_A(\Omega)\tilde{v}_m, \tilde{v}_m \rangle \end{pmatrix},$$

and using the relationship (9.1) between the \tilde{v}_j and the v_k we get that

$$\tilde{\Sigma}(dt) = D(t)^* \Sigma(dt) D(t), \quad (9.3)$$

where

$$D(t) := \begin{pmatrix} D_{11}(t) & \cdots & D_{m1}(t) \\ \vdots & \ddots & \vdots \\ D_{1n}(t) & \cdots & D_{mn}(t) \end{pmatrix}, \quad (9.4)$$

$D(t) : \mathbb{C}^m \rightarrow \mathbb{C}^n$.

Now since $A \in \text{Ext}(B_1)$, $B_1 \in \mathcal{S}_m(S)$, let $\mathcal{K} :=$ the cyclic subspace of L_Σ^2 generated by S and A . Let $U : L_\Sigma^2 \rightarrow L_\Sigma^2$ be defined by multiplication by $D(t)$, $V_A : \mathcal{K} \rightarrow \mathcal{K}_A$ be the model space isometry, and $W : L_\Sigma^2 \rightarrow \mathcal{K}_A$ be the deBranges Cauchy transform isometry.

Claim 9.4. *The linear map $U : L_\Sigma^2 \rightarrow L_\Sigma^2$ is an isometry which obeys*

$$V_A U = W, \quad \text{and} \quad U U^* = \mathbb{1}_{\mathcal{K}}.$$

Since U acts as multiplication by the matrix function $D(t)$, it is easy to see that U will intertwine $M^{\tilde{\Sigma}}$ and M^Σ . However we also want to verify that U takes the domain of $B \subset M_{\tilde{\Sigma}}$ into the domain of M_Σ . This claim will allow us to do this.

Proof. If $g \in L_\Sigma^2$ then the map $U : L_\Sigma^2 \rightarrow L_\Sigma^2$ defined by $Ug(t) = D(t)g(t)$ is clearly an isometry since

$$\|Ug\|^2 = \int_{-\infty}^{\infty} (D(t)^* \Sigma(dt) D(t)g(t), g(t)) = \|g\|^2.$$

Recall that \mathcal{K}_A is the space of Cauchy transforms of the measure $\tilde{\Sigma}$. The linear map V_A is an isometry from $K \subset L_\Sigma^2$ onto \mathcal{K}_A . We can extend V_A to a partial isometry acting on all of L_Σ^2 by the formula

$$V_A f(z) := \Omega_A(z)^* P_{\mathcal{K}} f = \tilde{J}^*(A - i)(A - z)^{-1} P_{\mathcal{K}} f = \tilde{J}^*(\mathcal{A} - i)(\mathcal{A} - z)^{-1} f,$$

for any $f \in L_\Sigma^2$. Then for any $f \in L_\Sigma^2$, $V_A f(z)$ is a column vector with components

$$(\Omega_A(z)^* f)_j = \int_{-\infty}^{\infty} \frac{t - i}{t - z} (\Sigma(dt) f(t), \tilde{v}_j(t)).$$

Since $\tilde{v}_j(t) = D_{j1}(t)v_1(t) + \dots + D_{jn}(t)v_n(t)$, it follows that the above can be written as

$$\begin{aligned} (\Omega_A(z)^* f)_j &= \int_{-\infty}^{\infty} \frac{t - i}{t - z} (D(t)^* \Sigma(dt) f(t), v_j(t))_{\mathbb{C}^m} \\ &= \frac{1}{i\pi} \int_{-\infty}^{\infty} \frac{1}{t - z} (D(t)^* \Sigma(dt) f(t), e_j)_{\mathbb{C}^m}, \end{aligned} \quad (9.5)$$

so that

$$V_A f(z) = \Omega_A(z)^* f = \frac{1}{i\pi} \int_{-\infty}^{\infty} \frac{1}{t - z} D(t)^* \Sigma(dt) f(t). \quad (9.6)$$

On the other hand the Cauchy transform isometry $W : L_\Sigma^2 \rightarrow \mathcal{K}_A$ obeys

$$Wg(z) = \frac{1}{i\pi} \int_{-\infty}^{\infty} \frac{1}{t - z} \tilde{\Sigma}(dt) f(t). \quad (9.7)$$

Finally, observe that for any $g \in L_\Sigma^2$,

$$V_A U g(z) = \frac{1}{i\pi} \int_{-\infty}^{\infty} \frac{1}{t - z} D(t)^* \Sigma(dt) D(t) g(t) = Wg(z).$$

This proves that

$$V_A U = W. \quad (9.8)$$

Now $U : L_\Sigma^2 \rightarrow L_\Sigma^2$ is an isometry, $V_A : L_\Sigma^2 \rightarrow \mathcal{K}_A$ is a partial isometry with initial space \mathcal{K} and $W : L_\Sigma^2 \rightarrow \mathcal{K}_A = \mathbf{L}(\tilde{\Phi}_A)$ is an onto isometry. If $\text{Ran}(U)$ is not contained in $\text{Ker}(V_A)^\perp$, then we could find an $f \in L_\Sigma^2$ such that $Uf = g_{\mathcal{K}} + g_\perp$ with $g_{\mathcal{K}} \in \mathcal{K}$ and $g_\perp \neq 0$ in $L_\Sigma^2 \ominus \mathcal{K}$. But then it would follow that

$$\|V_A U f\| = \|g_{\mathcal{K}}\| < \|f\|,$$

which would contradict the fact that

$$\|V_A U f\| = \|W f\| = \|f\|.$$

Hence

$$U = V_A^* V_A U = V_A^* W,$$

so that

$$U U^* = V_A^* W W^* V_A = V_A^* \mathbb{1}_{\mathcal{K}_A} V_A = \mathbb{1}_{\mathcal{K}}.$$

□

Now $WM_{\tilde{\Sigma}}W^* = \mathfrak{Z}_{\tilde{\Phi}_A}$ acts as multiplication by z in $\mathcal{K}_A = \mathbf{L}(\tilde{\Phi}_A)$. Also $V_AB_1V_A^*$ acts as multiplication by z in \mathcal{K}_A so that $V_AB_1 \subset \mathfrak{Z}_{\tilde{\Phi}_A}V_A$. This follows because $V_AB_1 = U_AB_1 = Z_AU_A$, where $Z_A = U_AB_1U_A^*$ acts as multiplication by z in $\mathcal{H}_A \subset \mathcal{K}_A$.

It follows that

$$U^*B_1 = W^*V_AB_1 \subset W^*\mathfrak{Z}_{\tilde{\Phi}_A}V_A = M_{\tilde{\Sigma}}U^*.$$

Now if $f \in \text{Dom}(B_1) \subset \text{Dom}(M_{\tilde{\Sigma}})$, then by the definition of the domain of $M_{\tilde{\Sigma}}$,

$$\int_{-\infty}^{\infty} \Sigma(dt)f(t) = 0.$$

We also have that $U^*f \in \text{Dom}(M_{\tilde{\Sigma}})$ so that

$$0 = \int_{-\infty}^{\infty} \tilde{\Sigma}(dt)D^{-1}(t)f(t) = \int_{-\infty}^{\infty} D^*(t)\Sigma(dt)f(t).$$

Alternatively if $B'_1 = M_{\tilde{\Sigma}}|_{U^*\text{Dom}(B_1)} \simeq B_1$, then for any $g \in \text{Dom}(B'_1)$ we have that $Ug \in \text{Dom}(M_{\tilde{\Sigma}})$ so that

$$\int_{-\infty}^{\infty} \tilde{\Sigma}(dt)g(t) = 0,$$

and

$$0 = \int_{-\infty}^{\infty} \Sigma(dt)D(t)g(t) = 0.$$

In summary we have established the necessity half of:

Theorem 9.5. *Let $B_1 \in \mathcal{S}_m(\mathcal{H}_1)$, $B_2 \in \mathcal{S}_n(\mathcal{H}_2)$ with characteristic functions Θ_1 and Θ_2 (where we fix a choice of Θ_2 to obey the condition of Remark (9.2)). If Θ_1 is inner then $B_1 \lesssim B_2$ if and only if the following three conditions hold:*

- (1) *There exists a contractive $\mathbb{C}^{m \times m}$ -valued analytic function Φ such that $\Phi \geq \Theta_1$.*
- (2) *The Herglotz measure $\tilde{\Sigma}$ of Φ is absolutely continuous with respect to the $\mathbb{C}^{n \times n}$ -valued Herglotz measure Σ of Θ_2 ,*

$$\tilde{\Sigma}(dt) = D^*(t)\Sigma(dt)D(t),$$

for a $\mathbb{C}^{m \times n}$ matrix-valued function $D(t)$ whose columns divided by $t + i$ belong to $L_{\tilde{\Sigma}}^2$.

- (3) *Suppose that $A \in \text{Ext}(B)$ is the extension such that $\Phi_A = \Phi$. If $\tilde{B}_1 := M_{\tilde{\Sigma}}|_{W^*V_A\text{Dom}(B_1)}$ where $W : L_{\tilde{\Sigma}}^2 \rightarrow \mathcal{K}_A$ is the deBranges isometry, then for any $f \in \text{Dom}(\tilde{B}_1)$ we have that*

$$\int_{-\infty}^{\infty} \tilde{\Sigma}(dt)f(t) = 0 \quad \text{and} \quad \int_{-\infty}^{\infty} \Sigma(dt)D(t)f(t) = 0.$$

Proof. To prove the sufficiency half of the above theorem, suppose that the above three conditions are satisfied and choose $A \in \text{Ext}(B_1)$ so that $\Phi_A = \Phi$ (such an A exists by Theorem 8.14).

We know that B_1 is unitarily equivalent to a restriction of $M_{\tilde{\Sigma}}$. Here are the details: Let $\tilde{\Sigma}$ be the matrix-valued measure which is π times the Herglotz measure for Φ_A . Let W be the Cauchy transform isometry which takes $L_{\tilde{\Sigma}}^2$ onto $\mathcal{K}_A = \mathbf{L}(\tilde{\Phi}_A)$ where $\tilde{\Phi}_A$ is the contractive analytic function corresponding to $\tilde{\Sigma}$. Then it is clear that $W^*V_AB_1 \subset W^*\mathfrak{Z}_{\tilde{\Phi}_A}V_A = M_{\tilde{\Sigma}}W^*V_A$. Let \tilde{B}_1 be the closure of $M_{\tilde{\Sigma}}$ restricted to $W^*V_A\text{Dom}(B_1)$.

Let U act as multiplication by $D(t)$. The second condition in the above theorem ensures that $U : L^2_{\Sigma} \rightarrow L^2_{\Sigma}$ is an isometry. The third condition in the above theorem ensures that this isometry $U : L^2_{\Sigma} \rightarrow L^2_{\Sigma}$ maps $\text{Dom}(\tilde{B}_1)$ into $\text{Dom}(M_{\Sigma})$ and since U acts as multiplication by $D(t)$, $U\tilde{B}_1 \subset M_{\Sigma}U$. In conclusion, $B_1 \simeq \tilde{B}_1 \lesssim M_{\Sigma} \simeq B_2$, so that $B_1 \lesssim B_2$. This proves the sufficiency of the above three conditions when Θ_1 is inner. \square

Remark 9.6. The technical assumption on the characteristic function Θ_2 from Remark 9.2 can be easily removed to obtain a fully general result:

Consider the Herglotz integral representation of the Herglotz function G_{Θ_2} :

$$\text{Re}(G_{\Theta_2}(z)) = P\text{Im}(z) + \int_{-\infty}^{\infty} \text{Re}\left(\frac{1}{i\pi} \frac{1}{t-z}\right) \Sigma_2(dt).$$

By Theorem 8.15, we see that there is a canonical self-adjoint extension $\mathfrak{Z}_{\Theta_2}(\mathbb{1})$ of \mathfrak{Z}_{Θ} such that $\Phi[\mathfrak{Z}_{\Theta_2}(\mathbb{1}); \mathfrak{Z}_{\Theta_2}] = \Theta_2$, and it follows that $P = \chi_{\{1\}}(b(\mathfrak{Z}_{\Theta_2}(\mathbb{1})))$. In particular if 1 is not an eigenvalue of the Cayley transform $U = b(\mathfrak{Z}_{\Theta_2}(\mathbb{1}))$ of $b(\mathfrak{Z}_{\Theta_2}(\mathbb{1}))$, then it follows from Section 4 that the deBranges Cauchy transform isometry $W_{\Theta_2} : L^2_{\Sigma_2} \rightarrow \mathbb{L}(\Theta_2)$ is onto. In this case, as in [4, Section 3.5, Section 5.4], one can check that W_{Θ_2} implements a unitary equivalence between \mathfrak{Z}_{Θ_2} and M_{Σ_2} , the symmetric operator of multiplication by t in $L^2_{\Sigma_2}$ on the domain

$$\text{Dom}(M_{\Sigma_2}) = \{f \in L^2_{\Sigma_2} \mid tf \in L^2_{\Sigma_2}; \int_{-\infty}^{\infty} \Sigma_2(dt)f(t) = 0\},$$

and moreover that W_{Θ_2} implements a unitary equivalence between $\mathfrak{Z}_{\Theta_2}(\mathbb{1})$, and M^{Σ_2} , the self-adjoint operator of multiplication by t in $L^2_{\Sigma_2}$.

By [2, Proposition 5.2.2], it follows that the canonical unitary extension $b(B(U))$ for $U \in \mathcal{U}(n)$ has 1 as an eigenvalue if and only if

$$\text{Ker}(\lim_{z \rightarrow 1} ((\Theta_B \circ b^{-1})(z)^* - U^*)) \neq \{0\},$$

where $z \in \mathbb{D}$ approaches 1 non-tangentially.

Note that in particular if B_2 is densely defined, then every canonical self-adjoint extension of B_2 is densely defined, and this happens if and only if no unitary extension of $b(B_2)$ has 1 as an eigenvalue, so that in this case $P = 0$, and W_{Θ_2} is onto. More generally the Livsic characteristic function Θ_2 of B_2 is really only defined up to conjugation by fixed unitary matrices. It follows that we can always fix a choice of Θ_2 so that $\mathfrak{Z}_{\Theta_2}(\mathbb{1})$ does not have 1 as an eigenvalue, so that $W_{\Theta_2} : L^2_{\Sigma_2} \rightarrow \mathbb{L}(\Theta_2)$ is an onto isometry, and we can assume without loss of generality that $B = M_{\Sigma_2}$. That is we fix a choice of Θ_2 so that

$$\text{Ker}(\lim_{z \rightarrow 1} ((\Theta_2 \circ b^{-1})(z)^* - U^*)) = \{0\}. \quad (9.9)$$

Alternatively, and perhaps more satisfactorily, it should be possible to remove the technical assumption from Remark 9.2 completely by re-expressing the conditions of the above Theorem in terms of spaces of square integrable functions on the unit circle, and the reproducing kernel Hilbert space on $\mathbb{C} \setminus \mathbb{T}$ obtained by taking the Cauchy transforms of such spaces. However as we have preferred to express our results in terms of L^2 spaces on the real line and Herglotz spaces on $\mathbb{C} \setminus \mathbb{R}$, we will not develop the necessary machinery to pursue this here.

Example 9.7. This example is a continuation of Example 8.10. Recall that we defined

$$V := \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},$$

$V \in \mathcal{V}_1(\mathbb{C}^2)$.

Now let

$$W := \begin{pmatrix} 0 & 3/5 & 4/5 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

It is straightforward to check that $W \in \mathcal{V}_1(\mathbb{C}^3)$, and that $W|_{\text{Ker}(V)^\perp} = V|_{\text{Ker}(V)^\perp}$. Also note that in Example 8.10 we defined

$$U := \begin{pmatrix} 0 & 3/5 & 4/5 \\ 1 & 0 & 0 \\ 0 & 4/5 & -3/5 \end{pmatrix}.$$

This is a unitary matrix, and moreover $U|_{\text{Ker}(W)^\perp} = W|_{\text{Ker}(W)^\perp}$, so that U is a unitary extension of W . Note however, that as shown in Example 8.10 that 1 is an eigenvalue of this choice of U . Hence in order to apply Theorem 9.5 we will instead work with a different canonical unitary extension of W . Let

$$X := \begin{pmatrix} 0 & 3/5 & 4/5 \\ 1 & 0 & 0 \\ 0 & -i4/5 & i3/5 \end{pmatrix}.$$

Then X is a canonical unitary extension of W and is hence also a unitary extension of $V \subseteq W$. As before let $B := b^{-1}(V)$, $T := b^{-1}(W)$ and $A := b^{-1}(X)$ so that $B \subset T \subset A$. Then $A \in \text{Ext}(T)$ is a canonical self-adjoint extension of T , and $A \in \text{Ext}(B)$ is a non-canonical extension of B and $B \lesssim T$. Let Θ_B and Θ_T be the characterisitic functions of B, T .

Our goal in this example is to verify that the three conditions of Theorem 9.5 are satisfied. Recall that

$$\Theta_B(z) = \left(\frac{z-i}{z+i} \right)^2,$$

and also recall that by Theorem 8.15, that since X is a canonical unitary extension of W , that up to a unimodular constant,

$$\Theta_T(z) = \Phi[A = b^{-1}(X); T](z).$$

Since Θ_T is only defined up to unimodular constants, we can and do fix $\Theta_T = \Phi[A; T]$. To show that the first condition of Theorem 9.5 is satisfied, we need to calculate $\Phi[A; B]$, and to verify that it is greater or equal to Θ_B . Recall that we did a similar calculation for the unitary matrix U which is a different unitary extension of W in Example 8.10.

We begin by calculating the Herglotz measure of $\Phi[A; B]$. Use that $\text{Ran}(V)^\perp = \text{Ker}(B^* + i)$ is spanned by e_1 , so that if σ_V is the Herglotz measure of $\phi[X; V] = \Phi[A; B] \circ b^{-1}$, that

$$\sigma_V(\Omega) = (e_1, P_X(\Omega)e_1).$$

Again this is a probability measure and $\left| (e_1, \hat{b}_2) \right| = \left| (e_1, \hat{b}_3) \right| =: a$ so that

$$1 = \sum_{k=1}^3 \left| (e_1, \hat{b}_k) \right|^2 = \frac{1}{6} + 2a,$$

$a = \frac{5}{12}$ and

$$\sigma_V = \frac{1}{6}\delta_i + \frac{5}{12}\delta_\lambda + \frac{5}{12}\delta_{-\bar{\lambda}}.$$

Finally as before

$$\Sigma_B = \pi \frac{1}{3}\delta_{-1} + \pi(1 + \beta^2)\frac{5}{12}\delta_\beta + \pi(1 + \beta^{-2})\frac{5}{12}\delta_{\beta^{-1}}.$$

As in Example 8.10, if $\Phi_A := \Phi[A; B]$ then

$$G_{\Phi_A}(z) = i\sigma_X(\{1\})z + \int_{-\infty}^{\infty} \frac{zt+1}{i(t-z)} \tilde{\sigma}_X(dt),$$

where $\tilde{\sigma}_X := \sigma_X \circ b$. Since 1 is not an eigenvalue of X , this becomes

$$G_{\Phi_A}(z) = -i \frac{1}{6} \frac{z-1}{z+1} - i \frac{5}{12} \frac{z\beta+1}{\beta-z} - i \frac{5}{12} \frac{z+\beta}{1-\beta z}.$$

Using that $\Phi_A = \frac{G_{\Phi_A}+1}{G_{\Phi_A}-1}$, and simplifying as in Example 8.10 shows that Φ_A is the product of three Blaschke factors with zeroes at the roots of the polynomial:

$$p(z) := 2(z-1)(\beta-z)(1-\beta z) + 5(z+1)(z\beta+1)(1-\beta z) + 5(z+1)(\beta-z)(1-\beta z) - 12i(z+1)(\beta-z)(1-\beta z).$$

It is a bit more tedious to calculate the roots of this polynomial this time. However it is not hard to check that $p(i) = 0$, and one can verify that p has a double root at $z = i$ and that the third root of p is located at the point $\mu = \frac{i-4}{i+4} \in \mathbb{C}_+$. It follows that up to a unimodular constant,

$$\Phi_A(z) = \left(\frac{z-i}{z+i} \right)^2 \frac{z-\mu}{z-\bar{\mu}},$$

which is indeed greater or equal to Θ_B .

We now show that the Herglotz measure of $\Phi[A; B](z)$, is absolutely continuous with respect to the Herglotz measure of $\Theta_T = \Phi[A; T]$ so that the second condition of Theorem 9.5 is also satisfied:

Let us calculate the Herglotz measure Σ_T of $\Theta_T = \Phi[A; T]$. Now $A = b^{-1}(X)$, and we calculate σ_X , the Herglotz measure of $\theta_X := \Theta_T \circ b^{-1}$, as in Example 8.10 by calculating the spectral measure of the unitary matrix X . The determinant of $(z - X)$ can be calculated to be

$$\det(z - X) = (z - i)(z - \lambda)(z + \bar{\lambda}) =: p(z), \quad \lambda := \frac{2}{5}\sqrt{6} - i\frac{1}{5}.$$

The eigenvectors \vec{b}_k , $1 \leq k \leq 3$ of X to the eigenvalues $\lambda_1 = i$, $\lambda_2 = \lambda$ and $\lambda_3 = -\bar{\lambda}$ are given by

$$\vec{b}_k := (1, \bar{\lambda}_k, \frac{5}{4}\lambda_k - \frac{3}{4}\bar{\lambda}_k)^T.$$

If $\hat{b}_k := \frac{\vec{b}_k}{\|\vec{b}_k\|}$, then one can check that

$$\hat{b}_1 = \frac{1}{\sqrt{6}}(1, -i, 2i).$$

The spectral measure of X is then

$$P_X := \sum_{k=1}^3 \left(\cdot, \hat{b}_k \right) \hat{b}_k \delta_{\lambda_k},$$

and since $v = e_3$ spans $\text{Ran}(W)^\perp = \text{Ker}(T^* + i)$,

$$\sigma_X(\Omega) = (e_3, P_X(\Omega)e_3).$$

Since P_X is unital, this means that σ_X is a probability measure so that

$$1 = \sum_{k=1}^3 |(e_3, \hat{b}_k)|^2 = \frac{2}{3} + |(e_3, \hat{b}_2)|^2 + |(e_3, \hat{b}_3)|^2.$$

Using that $\lambda_2 = \lambda = -\bar{\lambda}_3$, we get that $\|\vec{b}_2\| = \|\vec{b}_3\|$ and that $|(e_3, \hat{b}_2)| = |(e_3, \hat{b}_3)| =: a$ so that $1 = \frac{2}{3} + 2a$ and $a = \frac{1}{6}$. In conclusion,

$$\sigma_X = \frac{2}{3}\delta_i + \frac{1}{6}\delta_\lambda + \frac{1}{6}\delta_{-\bar{\lambda}}.$$

Now we use the fact that

$$\Sigma_T(\Omega) = \int_{\Omega} \pi(1+t^2)(\sigma_X \circ b)(dt),$$

to calculate that

$$\Sigma_T = \pi \frac{4}{3} \delta_{-1} + \pi(1+\beta^2) \frac{1}{6} \delta_\beta + \pi(1+\beta^{-2}) \frac{1}{6} \delta_{\beta^{-1}},$$

where $\beta := b^{-1}(\lambda)$. It follows that the Herglotz measure Σ_B of $\Phi[A; B]$ is indeed absolutely continuous with respect to the Herglotz measure Σ_T of $\Theta_T = \Phi[A; T]$.

Note that one can calculate that up to a unimodular constant

$$\Theta_T(z) = \frac{(z-i)(z-\mu_1)(z-\mu_2)}{(z+i)(z-\bar{\mu}_1)(z-\bar{\mu}_2)},$$

where

$$\mu_1 := i(4 + \sqrt{15}), \quad \text{and} \quad \mu_2 = i(4 - \sqrt{15}),$$

so that Θ_B is not a divisor of Θ_T .

Finally we verify that the third condition of Theorem 9.5 is satisfied. First we need to calculate the domain of $B = b^{-1}(V)$. We have that $\text{Ker}(V)^\perp$ is spanned by e_1 , and $\text{Dom}(B) = (1-V)\text{Ker}(V)^\perp$ so that $\text{Dom}(B)$ is spanned by the vector $(1, -1)$ (or if we view \mathbb{C}^2 as a subspace of \mathbb{C}^3 and $B \subset T$ then this is the vector $(1, -1, 0)$).

Let $\tilde{\Sigma} := \pi\Sigma_B$, and let $\Sigma := \pi\Sigma_T$. Let $\tilde{W} : L_{\tilde{\Sigma}}^2 \rightarrow \mathcal{L}(\tilde{\Phi}[A; B])$, and $W : L_{\Sigma}^2 \rightarrow \mathcal{L}(\tilde{\Phi}[A; T])$ be the corresponding deBranges isometries onto the Herglotz spaces. Also let $V_A : \mathbb{C}^2 \rightarrow \mathcal{L}(\tilde{\Phi}[A; B]) =: \tilde{\mathcal{K}}_A$, where $\tilde{\mathcal{K}}_A$ is the model reproducing kernel Hilbert space defined using the extension $A \in \text{Ext}(B)$ and $\Omega_A(z) := (A+i)(A-\bar{z})^{-1}\tilde{J}$ and $\tilde{J} : \mathbb{C} \rightarrow \text{Ker}(B^* + i)$ is defined by $\tilde{J}e_1 = e_1$ (here e_1 is a normalized basis vector for \mathbb{C}).

We need to calculate the image of $(1, -1)$ under the map \tilde{W}^*V_A which takes $\text{Dom}(B)$ into $\text{Dom}(M_{\tilde{\Sigma}})$:

$$\begin{aligned} (V_A(1, -1))(z) &= \Omega_A(z)^*(1, -1)^T \\ &= ((A-i)(A-z)^{-1}e_1, e_1) - ((A-i)(A-z)^{-1}e_2, e_1). \end{aligned}$$

Using that $e_2 = Xe_1$ where $X = b(A)$, we get this is

$$\begin{aligned}
(V_A(1, -1))(z) &= ((A - i)(A - z)^{-1}e_1, e_1) - ((A - i)(A - z)^{-1}(A - i)(A + i)^{-1}e_1, e_1) \\
&= \int_{-\infty}^{\infty} \frac{t - i}{t - z} (1 - b(t)) (P_A(dt)e_1, e_1) \\
&= \frac{1}{i\pi} \int_{-\infty}^{\infty} \frac{1}{t - z} \left(\frac{i}{\pi} \frac{1}{t + i} (1 - b(t)) \right) \tilde{\Sigma}(dt) \\
&= \tilde{W}f(z),
\end{aligned}$$

where $f \in L_{\Sigma}^2$ is

$$f(t) = (1 - b(t)) \frac{i}{\pi} \frac{1}{t + i}.$$

We can now verify that $f \in \text{Dom}(M_{\Sigma})$ by checking that $\int_{-\infty}^{\infty} \tilde{\Sigma}(dt)f(t) = 0$. This integral is equal to

$$\int_{-\infty}^{\infty} \tilde{\Sigma}(dt)f(t) = \frac{1}{3} \frac{1 - b(-1)}{-1 + i} + \frac{5}{12} (1 + \beta^2) \frac{1 - b(\beta)}{\beta + i} + \frac{5}{12} (1 + \beta^{-2}) \frac{1 - b(\beta^{-1})}{\beta^{-1} + i}.$$

Now using that $b(-1) = i$ and $b(\beta) = \lambda = -\frac{i}{5} + \frac{2}{5}\sqrt{6}$, this can be simplified to yield

$$\int_{-\infty}^{\infty} \tilde{\Sigma}(dt)f(t) = \frac{-1}{3} + \frac{5}{12} (2i\lambda - 2i\bar{\lambda}) = 0,$$

so that indeed $\tilde{W}^*V_A(1, -1)^T \in \text{Dom}(M_{\Sigma})$.

To verify the final condition of Theorem 9.5, we need to show that if $U_{\Sigma} : L_{\Sigma}^2 \rightarrow L_{\Sigma}^2$ is the isometry which acts as multiplication by $D(t)$ where

$$\tilde{\Sigma}(dt) = \overline{D(t)} \Sigma(dt) D(t),$$

then $U_{\Sigma}f \in \text{Dom}(M_{\Sigma})$. First we calculate $D(t)$ and U_{Σ} . We have by construction that

$$\tilde{\Sigma}(dt) = \pi^2 (1 + t^2) (P_A(dt)e_1, e_1),$$

and now observe that $Xe_1 = e_2$ and that $Xe_2 = 3/5e_1 - i4/5e_3 = 3/5X^*e_2 - i4/5e_3$. Rearranging this yields $e_2 = -i\frac{4}{5}(X^2 - 3/5)^{-1}Xe_3$ so that $e_1 = -i\frac{4}{5}(X^2 - \frac{3}{5})^{-1}e_3$, where recall that $X = b(A)$. It follows that

$$\begin{aligned}
(P_A(dt)e_1, e_1) &= \left(i\frac{4}{5}(b(A)^{-2} - 3/5)^{-1}P_A(dt)\frac{4}{5i}(b(A)^2 - 3/5)^{-1}e_3, e_3 \right) \\
&= \overline{D(t)} (P_A(dt)e_3, e_3) D(t),
\end{aligned}$$

with

$$D(t) = -i\frac{4}{5} \frac{1}{b(t)^2 - 3/5}.$$

Hence to complete the verification of the third condition of Theorem 9.5, we simply need show that if

$$g(t) := D(t)f(t) = \frac{4}{5\pi} \frac{1}{b(t)^2 - 3/5} \frac{1}{t + i} (1 - b(t)) \in L_{\Sigma}^2,$$

that

$$\int_{-\infty}^{\infty} \Sigma(dt)g(t) = 0.$$

Here is the calculation:

$$\begin{aligned}
\int_{-\infty}^{\infty} \Sigma(dt)g(t) &= \frac{4}{3} \frac{1}{i-3/5} \frac{1}{-1+i} (i-1) + \frac{1}{6} (1+b^{-1}(\lambda)^2) \frac{1}{\lambda-3/5} \frac{1}{\lambda+i} (\lambda-1) \\
&\quad + \frac{1}{6} (1+\beta^{-2}) \frac{1}{\bar{\lambda}^2-3/5} \frac{1}{b^{-1}(-\bar{\lambda})+i} (-\bar{\lambda}-1) \\
&= \frac{-5}{6} + \frac{1}{6} \frac{-2i\lambda}{\lambda^2-3/5} + \frac{1}{6} \frac{2i\bar{\lambda}}{\bar{\lambda}^2-3/5} \\
&= \frac{-5}{6} + \frac{i}{3} \left(\frac{\bar{\lambda}}{\bar{\lambda}^2-3/5} - \frac{\lambda}{\lambda^2-3/5} \right) \\
&= -\frac{5}{6} + \frac{i}{3} \frac{8}{5} \frac{\lambda-\bar{\lambda}}{|\lambda^2-\frac{3}{5}|^2} \\
&= 0.
\end{aligned}$$

In summary we have shown that if $f = \widetilde{W}^* V_A(-e_1 + e_2)$, where $\text{Dom}(B)$ is spanned by $-e_1 + e_2$, that both

$$\int_{-\infty}^{\infty} \widetilde{\Sigma}(dt)f(t) = 0 \quad \text{and} \quad \int_{-\infty}^{\infty} \Sigma(dt)D(t)f(t) = 0,$$

so that the third and final condition of Theorem 9.5 is satisfied.

10. OUTLOOK

There are several directions in which the results of this paper can be extended.

We have assumed throughout that $B \in \mathcal{S}$ has an inner Livsic characteristic function. A good portion of the theory we have developed here does not depend on this fact, and it would be good to generalize the results contained here to the case where the Livsic function is an arbitrary contractive analytic function (vanishing at $z = i$). We have done some work on this already, in particular Example 4.6 can be generalized to show that if $\Theta \leq \Phi$ are arbitrary contractive analytic functions that there is a bounded multiplier $V : L(\Theta) \rightarrow L(\Phi)$ which intertwines \mathfrak{Z}_Θ and \mathfrak{Z}_Φ . However it is not clear whether $\mathfrak{Z}_\Theta \lesssim \mathfrak{Z}_\Phi$ in this general case, or whether more general definitions of partial order, and extensions of a symmetric linear transformation are needed. Also if $A \in \text{Ext}(B)$ where Θ_B is not inner, then one can show that in general \mathcal{H}_A is only boundedly contained in \mathcal{K}_A , and so is not just a Hilbert subspace. Once these results are successfully generalized to arbitrary simple symmetric and isometric linear transformations with equal indices, a natural question is whether our partial order results can be extended to arbitrary contractions. Namely given contractions T_1, T_2 , perhaps one could define that $T_1 \lesssim T_2$ if $T_1 \simeq T'_1 \subseteq T_2$. Perhaps this could be accomplished by using the fact that the problem of unitary equivalence of contractions is equivalent to the problem of unitary equivalence of partial isometries, see [6, Theorem 1] and the discussion following it.

There should be several interesting consequences of the results already obtained in this paper. For example as discussed in Remark 7.4, we can use the theory developed here to provide an alternate proof of the Alexandrov isometric measure theorem, [17, Theorem 2]. In fact the result we obtain is a generalization of the operator theoretic result of Krein [5, Chapter 1, Corollary 2.1] which uses the theory of entire symmetric operators and hence holds for the case where Θ_B is a meromorphic scalar-valued inner function. We point out that this result of Krein can be used to prove the

Alexandrov isometric measure theorem, and that de Branges has also proven this result in the case where Θ is meromorphic in his book [12, Theorem 32]. Our generalization holds for arbitrary inner functions, and it should be possible to extend this to vector-valued Hardy spaces and matrix-valued inner functions as well. Our theory should also allow us to extend the main result of [23] to the case of arbitrary inner functions and nearly invariant subspaces, as well as to vector-valued versions of nearly invariant subspaces.

Finally as discussed in Remark 8.6, there is a natural bijection between the sets $\text{Ext}(B)$ and $\text{POVM}(B)$, the set of all unital positive operator valued measures which diagonalize B . It is easy to see with an application of Naimark's dilation theorem that $\text{POVM}(B)$ is a convex set, and we think it could be interesting to study the properties of this convex set, for example to determine its extreme points, and to study its Choquet theory. It is known that $\text{POVM}(B)$ is a face in the set of all unital positive-operator valued measures on \mathbb{R} [24, Theorem 13.6.3], and consequently that every projection valued measure corresponding to a canonical $A \in \text{Ext}(B)$ is an extreme point of this set (although this can be proven directly). Naimark has proven that if $B \in \mathcal{S}_n(\mathcal{H})$ and $A \in \text{Ext}(B)$ is self-adjoint in \mathcal{K} where $\mathcal{K} \ominus \mathcal{H}$ is finite dimensional, then the positive operator-valued measure corresponding to A is an extreme point of $\text{POVM}(B)$ [25]. Moreover Gilbert has proven that if $B \in \mathcal{S}_n(\mathcal{H})$, then the set of all $Q \in \text{POVM}(B)$ which correspond to $A \in \text{Ext}(B)$ defined on \mathcal{K} with $\mathcal{K} \ominus \mathcal{H}$ finite dimensional is dense in a natural topology on $\text{POVM}(B)$ [26]. It could be interesting to see whether the extreme points of $\text{POVM}(B)$ can be given a function theoretic characterization in terms of the characteristic functions $\Phi[A; B]$ of the corresponding extensions of B .

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